scientific reports

Check for updates

OPEN

Optimization of separation and purification processes in diethyl ether production for improved efficiency and sustainability

Amin Hedayati Moghaddam[1]✉ & Morteza Esfandyari[2]

This study focuses on optimizing the separation and purification processes in diethyl ether (DEE) production to enhance energy efficiency, reduce waste, and improve product quality. Utilizing process simulation with Aspen-Hysys-V14, statistical modeling, and optimization techniques, this study investigates operational parameters across key units, including two drums and two distillation columns. Design of experiment was performed using response surface methodology (RSM) and central composite design (CCD). Key results indicate that under optimized conditions, a DEE purity of 96.43% was achieved with total energy consumption of 2,150,566 kJ/h, corresponding to an energy requirement of 1,499,754.87 kJ/kmol of DEE. Scenario-based optimization minimized DEE loss in fuel and vent streams while balancing energy demands. Non-linear relationships between parameters, such as temperature and pressure, were modeled with high predictive accuracy. These findings contribute to the development of sustainable and cost-effective DEE production processes and offer transferable insights for similar chemical manufacturing systems.

Keywords Diethyl ether, Energy efficiency, Sustainability, Process optimization

Diethyl ether (DEE) is an organic compound widely used in industrial and scientific applications. Its properties, such as high volatility, low boiling point, and excellent solvent capabilities, make it a critical component in biodiesel production[1–3], fuel additives[4], and laboratory processes. In fuel formulations, it is utilized to enhance combustion efficiency[5,6]. These diverse applications underscore the importance of optimizing the production of DEE to meet growing industrial demands. DEE is primarily produced through the catalytic dehydration of ethanol, a process that involves precise control of operational parameters to maximize DEE yield while minimizing byproducts such as ethylene. This production route has gained increased attention due to its potential for utilizing bioethanol derived from renewable resources[7], offering a sustainable alternative to fossil fuel-based chemical production. Optimizing DEE production not only meets the efficiency and economic goals but also aligns with global efforts toward green and sustainable industrial practices.

In a typical production process, ethanol is converted to DEE in a dehydration reactor under specific temperature and pressure conditions. The reactor output contains DEE, unreacted ethanol, water, and byproducts, which must be separated and purified to obtain high-purity DEE suitable for industrial use. The separation section includes a combination of physical and thermal processes, such as distillation and liquid-gas separation, to isolate DEE from other components in the reaction mixture. The design and operation of these processes must strike a delicate balance between minimizing fixed capital investment and operational cost, maximizing product recovery, and minimizing energy consumption. For instance, increasing the number of distillation stages can improve the separation efficiency but may also lead to higher energy requirements and higher fixed capital investment. Similarly, operating at elevated pressures can enhance product purity but may impose additional demands on equipment and energy resources. The separation and purification section, therefore, plays a pivotal role in determining the overall efficiency and sustainability of the production process. It consists of multiple interconnected units, including distillation columns, two phase drums, pumps, and heater and coolers. Each of which influences both the product quality and the energy consumption of the system.

The separation and purification section not only ensures the desired product purity but also offers significant opportunities for reducing energy consumption and operational costs. Factors such as distillation column design, operating temperatures, pressures, and the number of separation stages can substantially affect the

[1]Department of Chemical Engineering, CT.C., Islamic Azad University, Tehran, Iran. [2]Department of Chemical Engineering, University of Bojnord, Bojnord, Iran. ✉email: Ami.hedayati_moghaddam@iau.ac.ir

energy efficiency and overall performance of the process. To address these challenges, selecting a systematic approach to optimizing the separation and purification section is essential. This involves not only understanding the fundamental principles governing separation processes but also applying advanced tools and methodologies to analyze and improve system performance.

Simulation and modeling of chemical processes play an important role in understanding, optimizing, and predicting the behavior of complex systems in industries such as petrochemicals and energy. Several methods are employed for this purpose, including kinetics models[8], statistical approach[9,10], and machine learning models[11–16], as well as process simulation tools like Aspen-Hysys[17–21]. These approaches make possible the advancements in technology and sustainability. Process simulation software, such as Aspen-Hysys, provides a powerful platform for modeling complex chemical processes and evaluating the effects of various operating conditions. By simulating the behavior of the separation and purification system under different scenarios, it is possible to identify key factors and explore strategies for finding optimum conditions. There are several studies applied Aspen-Hysys to simulate the separation and purification section in different chemical production process[22,23].

Statistical techniques such as response surface methodology (RSM) offer a structured framework for investigating the effects of multiple operational parameters simultaneously[24–29]. These methodologies allow for the development of predictive models that capture the relationships between input variables and performance metrics, such as DEE purity and energy consumption. By analyzing the interactions and quadratic effects of parameters, these models provide valuable insights into the relations between operational parameters and the performance of separation and purification system.

Optimization of the separation and purification section requires a perspective that considers both technical and economic factors. On the technical side, achieving high product purity is essential to meet industrial quality standards and minimize material losses. On the economic side, reducing energy consumption and operational costs is crucial for enhancing the profitability and sustainability of the production process. These objectives are often interdependent, requiring a careful balance to achieve optimal results. For example, operating a distillation column at higher temperatures may improve separation performance but also increase energy consumption. So, making a comprehensive evaluation of cost-benefit trade-offs is necessary.

The main step in the optimization process involves the application of optimization functions such as desirability function (DF), genetic algorithm (GA) etc. to identify the optimal set of operating conditions. DF provides a mathematical approach to balancing multiple objectives, such as maximizing product purity while minimizing energy consumption. By defining different scenarios and strategies, this approach ensures that the optimization results is in agreement with specific production goals and constraints.

The current study aims to address this gap by focusing on the separation and purification section of DEE production. The objectives are to investigate the performance of the separation and purification system in terms of product purity and waste minimization. Further, to identify areas for improvement, the energy consumption across the separation units, including distillation columns and drums were analyzed. The effects of key operational parameters, such as temperature and pressure on separation efficiency and energy usage were examined. Several statistical models were developed to capture the relationships between operational parameters and performance metrics. Using the developed models, sensitivity analysis was performed to understand the influence of individual parameters and their interactions on process performance. Finally, the separation and purification section were optimized to achieve a balance between energy efficiency and product quality. By improving the energy efficiency and sustainability of DEE production, this research contributes to broader efforts to reduce the environmental footprint of chemical manufacturing. The insights gained from this study can also be applied to other chemical processes involving similar separation challenges. So, this work is a valuable contribution to the field of process engineering.

Methods and materials

This study employs a systematic approach that combines process simulation, statistical modeling, and optimization of four separation units including two drums and two distillation columns to achieve the stated objectives. In this approach, each separation unit is examined and optimized from technical and economical perspectives.

Process description

Figure 1 shows the process flow diagram (PFD) of separation and purification section of DEE production. This section of process is a multi-step operation aimed at separating and purifying DEE from the output of the reaction section. The output of reaction section is a mixture of DEE, unreacted ethanol, water, and byproducts such as ethylene. The purification process begins with the mixture entering drum1. In this drum, gas-liquid separation occurs. The gaseous phase, which includes minor DEE, is vented, and the liquid phase proceeds to further stages. Temperature in drum1 is controlled via a heat exchanger, and pressure is regulated using a pressure-reducing valve. After the initial separation, the liquid is sent to distillation column1 for primary distillation. This column separates heavier impurities from DEE by using precise adjustments of operational parameters. The top stream of this column, partially purified DEE, is transferred to the next stage, while heavier components are entered into bottom stream.

The bottom stream of distillation column1 is fed into distillation column2 for separating unreacted ethanol. The top stream of column2 is recycled to reaction section and bottom stream is wasted. The top stream of column1 enters drum 2, where the residual gas is separated from the liquid product. This ensures that the final product has the desirable purity. The purified DEE exiting drum 2 is the final product and is ready for industrial use.

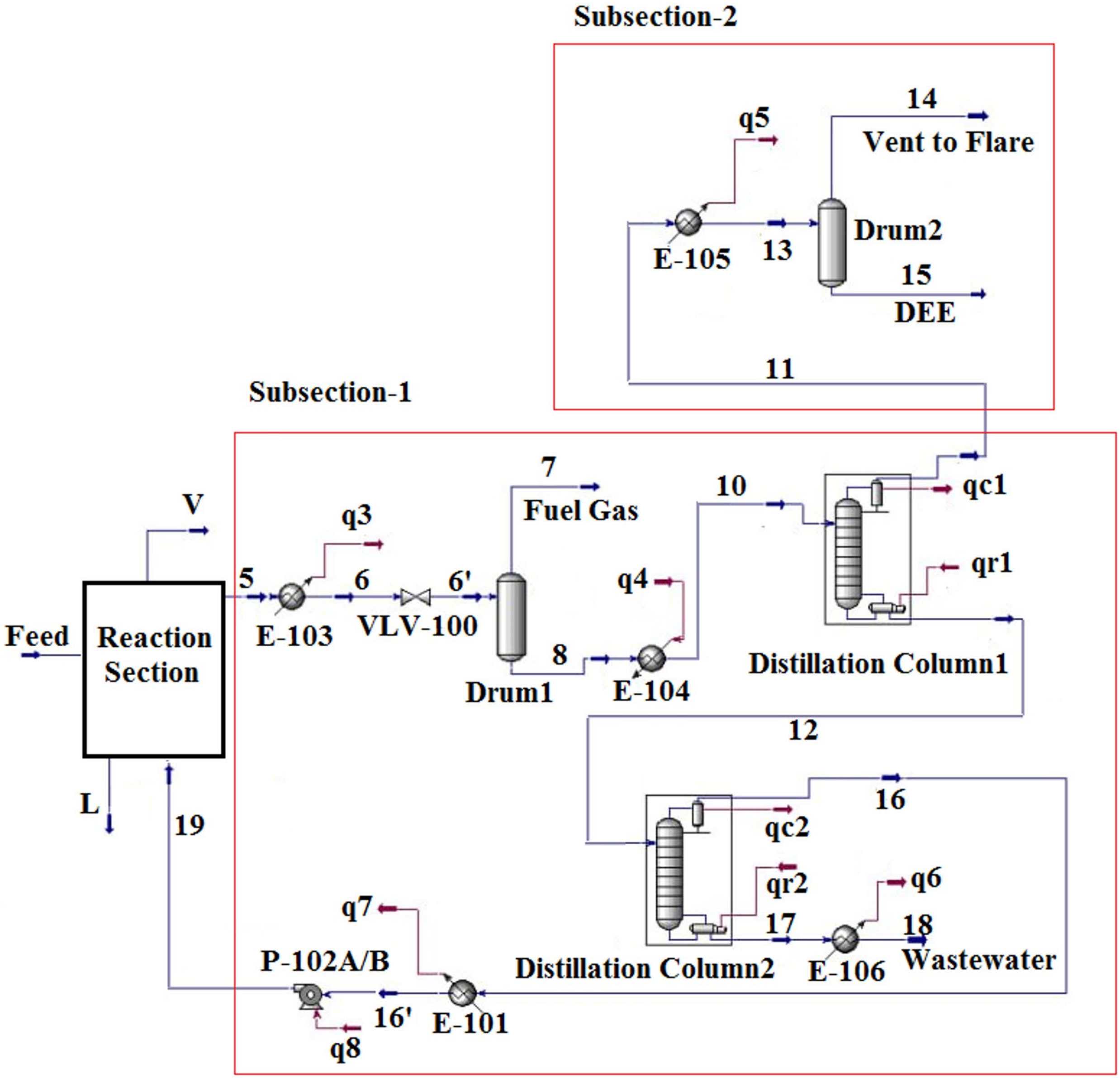

Fig. 1. Process flow diagram (PFD) of separation and purification section in DEE production process.

Thermodynamic model selection

In Aspen-Hysys-V14 simulation, the non-random two-liquid (NRTL) model was selected as the thermodynamic model to represent the behavior of mixture. By using NRTL within simulation, vapor-liquid equilibrium (VLE), liquid-liquid equilibrium (LLE), and other non-ideal phenomena can be modeled. This results in more accurate process simulations, better design decisions, and improved operational strategies.

Experimental design

Several units are included in the separation section, and the performance of each unit affects the others. Therefore, this section was divided into two subsections, termed 1 and 2, and each subsection was investigated separately. Subsection 1 includes drum1, distillation column1, and distillation column2. Subsection2 includes drum2.

Using RSM and central composite design (CCD) techniques, a structured experimental design is developed for each subsection. RSM-CCD ensures efficient exploration of the operational parameter space while minimizing the number of required simulations runs. Key parameters to be investigated and their operational ranges for each subsection have been presented in Table 1.

Statistical modeling

The data generated from the simulations will be used to develop statistical models that describe the relationships between operational parameters and outputs, such as DEE purity and energy consumption. Several models such as linear, two-factor interaction (2FI), and polynomial are investigated and the best fitted model is

	Independent Variable	Sign	Unit	Operational Range
Subsection1	Inlet Temperature-D1	A	°C	15–40
	Inlet Temperature-C1	B	°C	40–70
	Pressure-C1	C	kPa	100–300
	Inlet Temperature-C2	D	°C	95–120
	Pressure-C2	E	kPa	50–100
Subsection2	Inlet Temperature-D2	F	°C	5–30
	Pressure-D2	G	kPa	30–88

Table 1. Operational range of independent variables.

	Source	Sum of Squares	df	Mean Square	F-value	*p*-value	
Cooler Energy Consumption	**Model**	5.292E + 09	2	2.646E + 09	95.36	< 0.0001	significant
	A-Temperature-D1	1.693E + 09	1	1.693E + 09	61.01	< 0.0001	
	E-Pressure-C2	3.599E + 09	1	3.599E + 09	129.72	< 0.0001	
	Residual	1.110E + 09	40	2.775E + 07			
	Cor Total	6.402E + 09	42				
DEE Flowrate	**Model**	0.0200	7	0.0029	4949.28	< 0.0001	significant
	A-Temperature-D1	0.0197	1	0.0197	34145.94	< 0.0001	
	B-Temperature-C1	7.384E-07	1	7.384E-07	1.28	0.2652	
	E-Pressure-C2	0.0001	1	0.0001	156.37	< 0.0001	
	AE	4.880E-06	1	4.880E-06	8.47	0.0062	
	BE	6.120E-06	1	6.120E-06	10.63	0.0025	
	A^2	0.0002	1	0.0002	317.96	< 0.0001	
	E^2	2.171E-06	1	2.171E-06	3.77	0.0603	
	Residual	0.0000	35	5.759E-07			
	Cor Total	0.0200	42				

Table 2. ANOVA for DEE flowrate in fuel stream and cooler energy consumption of drum1.

selected for each unit. These models will be validated using metrics such as R^2, adjusted R^2, and predicted R^2 to ensure accuracy and reliability. Further, analysis of variance (ANOVA) was performed to explore the degree of importance of each factor and their interactions.

Results and discussion

In previous study, the ethanol dehydration reaction was simulated and optimized from both technical and economic perspectives[30]. In the current study, the process was first run based on the reactor optimum conditions obtained in the previous work. Next, the separation and purification section are investigated, simulated, and optimized.

Subsection1

Drum1

The first unit in subsection1 is drum1. The placement of a drum downstream of the reactor is due to the presence of a two-phase fluid within the pipeline. Specifically, the drum functions to separate and remove the gas phase, which is subsequently vented. The objective of this optimization is to determine conditions that minimize the release of DEE into the atmosphere. The temperature and pressure of drum are set using a heat exchanger and a pressure reducing valve.

Table 2 presents the ANOVA for two critical metrics in drum1: cooler energy consumption and DEE flowrate in the vent stream. These outputs are essential for optimizing the efficiency of the separation process in this unit. Cooler energy consumption refers to the energy required to regulate the temperature of the stream before entering drum1, while the DEE flowrate in the vent stream indicates the amount of DEE loss to the atmosphere. The ANOVA results reveal that temperature of drum1 (A) and the pressure of column2 (E) are the most influential factors for both metrics, showing the highest F-values and statistical significance ($p < 0.0001$). For DEE flowrate, the squared term of temperature of drum1 (A^2) also demonstrates significant non-linear effects. This highlights the complexity of temperature role in DEE flowrate. Additionally, the interaction between AE and BE influence the DEE flowrate. This issue showcases the interdependence of these variables.

The Eqs. 1 and 2 derived from the obtained data provide a mathematical representation of the relationships between input and output parameters. Note, the DEE flowrate equation captures the effects of temperature of drum1 and column1, pressure of column2, and their interactions, while the energy consumption equation focuses on the influence of temperature of drum1 and pressure of column2. These equations are pivotal for

	Std. Dev.	Mean	C.V. %	Adeq Precision	R^2	Adjusted R^2	Predicted R^2
Cooler Energy Consumption	5267.58	4.647E+05	1.13	31.1660	0.8266	0.8180	0.7965
DEE Flowrate	0.0008	0.1010	0.7516	309.6446	0.9990	0.9988	0.9982

Table 3. Specifications of statistical models for predicting DEE flowrate and cooler energy consumption in drum1.

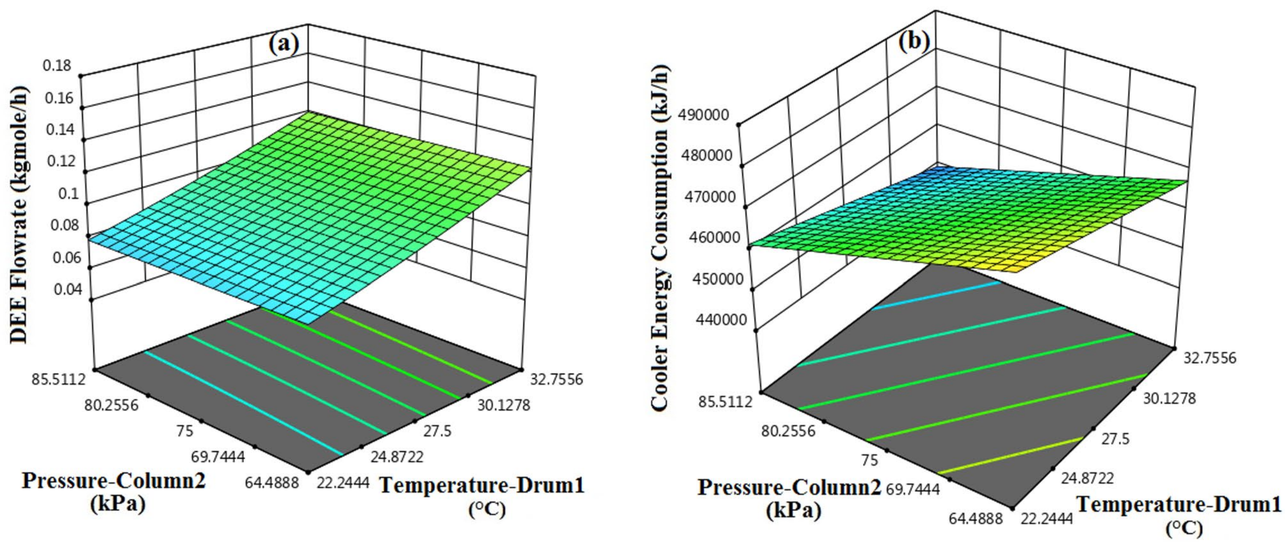

Fig. 2. Effects of temperature and pressure on DEE flowrate and cooler energy consumption in drum1.

optimizing the operational parameters, reducing energy consumption, and minimizing DEE loss. So, these models are useful in improving the overall efficiency and sustainability of the production process.

$$\text{DEE Flowrate} = +0.0988 + 0.0213 \times \text{A} - 0.0001 \times \text{B} - 0.0014 \times \text{E} - 0.0004 \times \text{AE} + +0.0004 \times \text{BE} + 0.0019 \times \text{A}^2 + 0.0002 \times \text{E}^2 \quad (1)$$

$$\text{Energy Consumption} = +4.647\text{E} + 05 - 6251.53 \times \text{A} - 9115.93 \times \text{E} \quad (2)$$

Table 3 presents the specifications of the developed models. The introduced metrics evaluate the statistical robustness and reliability of the models. The Adjusted R^2 for both models is slightly lower than the R^2. The predicted R^2 is a measure of how well the model can predict new data that were not used to fit the model. It gives an indication of the model predictive accuracy. The predicted R^2 value for cooler energy consumption and DEE flowrate are 0.7965 and 0.9982, respectively. These values indicate a very high predictive accuracy. So, these models can reliably predict energy consumption and DEE loss based on input parameters Further, the low coefficient of variation (C.V.%) for both models highlights their high precision. This information validates the use of these models for optimizing operational parameters, which are critical for reducing energy consumption and minimizing DEE loss.

Figure 2 examines energy consumption and DEE loss in drum1. Figure 2a shows that as temperature-D1 increases, the DEE flowrate in the vent stream rises significantly. This suggests that elevated temperatures enhance the vaporization of DEE, leading to increased losses through the vent. Additionally, increasing pressure-C2 reduces DEE flowrate in the vent stream, slightly. It is clear that the effect of pressure-C2 is negligible. Figure 2b shows that by decreasing the temperature-D1, energy consumption increases due to the increased cooling demand required to maintain process temperature. This trend suggests that lower temperatures drastically increase operational costs.

Distillation column1

Following the optimization of drum1, the focus shifts to modeling and optimizing the separation performance and energy efficiency of distillation column1. This involves examining the effects of the selected operational parameters. Figure 3 shows the composition of top stream leaving the distillation column for different operational conditions at different runs. It is obvious that there is no considerable change in composition. So, the focus shifts only to minimizing the energy consumption.

Table 4 presents the ANOVA for energy consumption related to this column. The energy consumption in heater E-104 and reboiler were modeled. It is worthwhile noting that a reliable model for predicting energy consumption in condenser was not extracted from the obtained data. For heater, the model is highly significant.

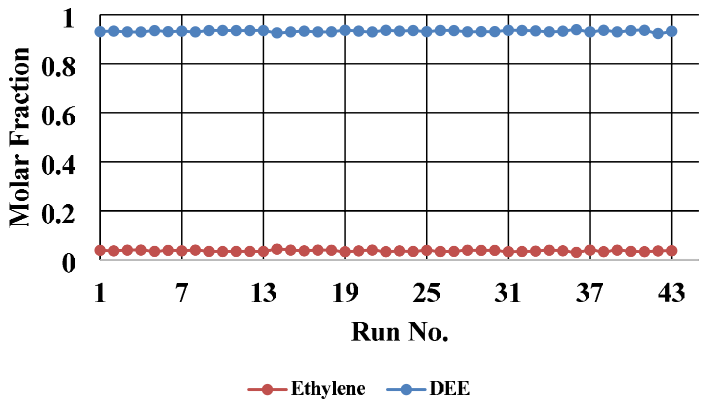

Fig. 3. Composition of the top stream in distillation column1 under varying operational conditions.

	Source	Sum of	Mean	F-value	*p*-value	Description
	Model	3.672E+10	6	6.119E+09	3674.92	<0.0001
	A-Temperature-D	1.620E+09	1	1.620E+09	973.04	<0.0001
	B-Temperature-C1	1.930E+10	1	1.930E+10	11590.52	<0.0001
	C-Pressure-C1	1.497E+10	1	1.497E+10	8989.06	<0.0001
Heater	BC	6.981E+08	1	6.981E+08	419.25	<0.0001
	B^2	8.676E+07	1	8.676E+07	52.10	<0.0001
	C^2	1.840E+07	1	1.840E+07	11.05	0.0020
	Residual	5.995E+07	36	1.665E+06		
	Cor Total	3.678E+10	42			
	Model	4.167E+10	3	1.389E+10	633.48	<0.0001
	B-Temperature-C1	1.782E+10	1	1.782E+10	812.90	<0.0001
Reboiler	C-Pressure-C1	2.343E+10	1	2.343E+10	1068.67	<0.0001
	BC	4.138E+08	1	4.138E+08	18.87	<0.0001
	Residual	8.550E+08	39	2.192E+07		
	Cor Total	4.252E+10	42			

Table 4. ANOVA for reduced models developed for energy consumption in different units of distillation column1.

The inlet temperature of column1 (B) and pressure of column1 (C) have very high F-value and an extremely low p-value. This indicates that temperature and pressure are major factors influencing heater energy consumption. Temperature of drum1 (A), with an F-value of 973.04, is also significant, but less so than B and C. Further, BC, B^2, and C^2 are significant factor. This implies that non-linear effects also matter in heater energy consumption. It is important to note that the significance of BC is higher than B^2 and C^2. For reboiler, B, C, and their interactions have significant effects on energy consumption. The values of predicted R2 for heater and reboiler are 0.9961 and 0.9744, respectively. These high values indicate high preciseness of the developed models.

Figure 4 illustrates the energy consumption patterns for the heater and reboiler in distillation column1 as a function of key operational parameters. Figure 4a shows a strong dependence of heater duty on the temperature of column1 and its pressure. Increased temperature and decreased pressure values lead to significant energy demands for heater. Figure 4b shows that reboiler energy consumption rises with decreasing inlet temperature and increasing pressure in column 1. This observation implies the need for careful calibration of these parameters.

Distillation column2

Table 5 presents the results of ANOVA for energy consumption in condenser and reboiler of culmn2. The energy consumption in the condenser is significantly influenced by the pressure of column2 (E), which has the highest influence (F-value of 118.87) and in less extent by pressure of column1 (C). The energy consumption in reboiler is predominantly determined by pressure in column2 (E). Elevated pressure enhances the boiling point of the mixture. This requires greater energy input to maintain operational efficiency. The predicted R2 of these two models are 0.71 that have less preciseness in comparison with previous models.

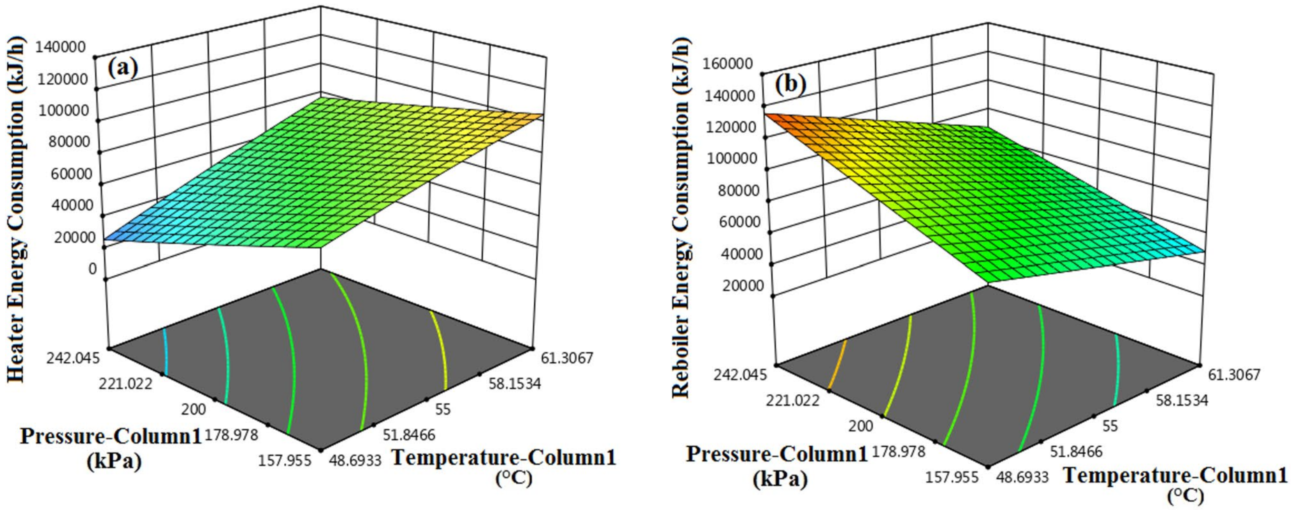

Fig. 4. Energy consumption in heater and reboiler of distillation column 1 as a function of key operational parameters.

	Source	Sum of Squares	df	Mean Square	F-value	p-value	
Condenser	**Model**	1.120E + 08	6	1.866E + 07	28.89	< 0.0001	significant
	B-Temperature-C1	2428.55	1	2428.55	0.0038	0.9515	
	C-Pressure-C1	1.190E + 07	1	1.190E + 07	18.42	0.0001	
	E-Pressure-C2	7.680E + 07	1	7.680E + 07	118.87	< 0.0001	
	BC	4.598E + 06	1	4.598E + 06	7.12	0.0114	
	BE	9.952E + 06	1	9.952E + 06	15.40	0.0004	
	E^2	8.731E + 06	1	8.731E + 06	13.51	0.0008	
	Residual	2.326E + 07	36	6.461E + 05			
	Cor Total	1.352E + 08	42				
Reboiler	**Model**	2.051E + 10	1	2.051E + 10	118.65	< 0.0001	significant
	E-Pressure-C2	2.051E + 10	1	2.051E + 10	118.65	< 0.0001	
	Residual	7.087E + 09	41	1.729E + 08			
	Cor Total	2.759E + 10	42				

Table 5. ANOVA for energy consumption in reboiler and condenser of distillation column2.

Scenario No.	Temperature-D (°C)	Temperature-C1 (°C)	Pressure-C1 (kPa)	Temperature-C2 (°C)	Pressure-C2 (kPa)	Total Energy Consumption (kJ/h)	DEE Flowrate-Fuel Stream (kgmole/h)
I	**31.213**	**40.000**	**132.806**	**96.541**	**55.500**	**1,255,110**	**0.116**
II	**38.674**	**40.000**	**125.491**	**104.368**	**53.181**	**1,224,632**	**0.155**

Table 6. Optimum conditions for subsection 1 under different scenarios.

Optimization-subsection1

Table 6 presents the results of performing optimization for subsection1. Two scenarios were considered for optimizing the performance of this subsection. Scenario I emphasizes achieving the lowest DEE flowrate in the fuel stream and energy consumption. This scenario aims to improve economic efficiency and align with sustainable practices. Scenario II prioritizes minimizing the energy consumption to reduce operational costs, while the DEE flowrate in the fuel stream is considered within the acceptable range. So, slightly higher DEE loss is observed compared to Scenario I.

Subsection2

After adjusting the values of operational parameters of subsection1, the subsection2 is investigated and examined. The main unit in this subsection is drum2. For this unit, two operative parameters are selected and their effects

	Source	Sum of Squares	df	Mean Square	F-value	*p*-value	
DEE Flowrate	**Model**	4.16	4	1.04	68.55	< 0.0001	significant
	F-Temperature-D2	1.82	1	1.82	119.69	< 0.0001	
	G-Pressure-D2	1.85	1	1.85	121.91	< 0.0001	
	F^2	0.2746	1	0.2746	18.08	0.0028	
	G^2	0.2848	1	0.2848	18.75	0.0025	
	Residual	0.1215	8	0.0152			
	Cor Total	4.29	12				
Cooler Energy Consumption	**Model**	5.079E + 09	4	1.270E + 09	77.67	< 0.0001	significant
	F-Temperature-D2	2.552E + 09	1	2.552E + 09	156.13	< 0.0001	
	G-Pressure-D2	2.005E + 09	1	2.005E + 09	122.65	< 0.0001	
	F^2	2.752E + 08	1	2.752E + 08	16.83	0.0034	
	G^2	3.144E + 08	1	3.144E + 08	19.23	0.0023	
	Residual	1.308E + 08	8	1.635E + 07			
	Cor Total	5.210E + 09	12				

Table 7. ANOVA for DEE flowrate in vent stream and cooler energy consumption in drum2.

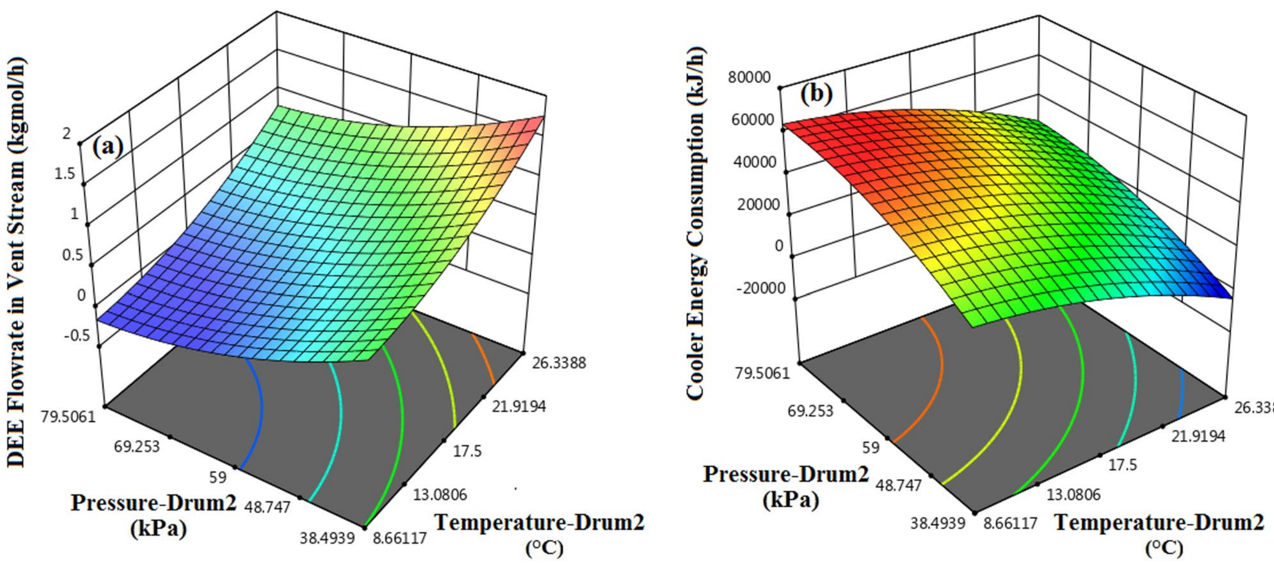

Fig. 5. Effects of temperature and pressure on DEE flowrate and cooler energy consumption in drum2.

on DEE flow rate in the vent stream and energy consumption in cooler-E105 are investigated. Table 7 presents the results of an ANOVA conducted on the operational parameters of Drum 2 in the DEE separation process. Both temperature (F) and pressure (G) of Drum 2 significantly influence the DEE flow rate, with F-values of 119.69 and 121.91, respectively. The squared terms of these parameters (F^2 and G^2) also highlight non-linear relationships between these factors and the DEE flow rate. Similarly, temperature and pressure significantly affect the cooler energy consumption, with high F-values (156.13 for temperature and 122.65 for pressure). With p-values < 0.01, non-linear effects (F^2 and G^2) also play a significant role in energy consumption of cooler.

With R^2 values of 0.9717 for DEE flow rate and 0.9749 for cooler energy consumption, the developed models demonstrate excellent statistical robustness. Predicted R^2 values are slightly lower (0.8696 for DEE flow rate and 0.8840 for cooler energy consumption). These values of predicted R2 reflect strong predictive capabilities.

Figure 5a shows as temperature increases, the DEE flow rate in the vent stream rises significantly. This indicates that higher temperatures enhance the vaporization of DEE. This results in increased loss through the vent. Further, an increase in pressure reduces the DEE flow rate in the vent stream. This occurs because higher pressure suppresses vaporization. So, more DEE retains in the liquid phase. According to Fig. 5b, as temperature decreases, cooler energy consumption rises. This is because maintaining lower temperatures requires more energy for cooling.

The trends in Fig. 5(a) and Fig. 5(b) highlight the trade-off between minimizing DEE losses and reducing energy consumption. It is obvious that lower temperatures and higher pressures reduce DEE loss but demand more energy for cooling. Optimizing operational conditions involves balancing these parameters to achieve sustainable and cost-efficient performance. To perform this, two scenarios were defined. In scenario 1, the values

Scenario No.	Temperature-D2	Pressure-D2	Cooler Energy Consumption	DEE Flowrate in Vent Stream
1	26.067	87.990	28728.510	0.778
2	29.971	53.115	184.017	1.628

Table 8. Optimum conditions for drum2 under different scenarios.

Stream Name	Mol. Fraction			
	DEE	Ethanol	Ethylene	Water
Feed	0.0000	0.8880	0.0000	0.1120
V	0.0000	0.6402	0.0000	0.3598
L	0.0034	0.0189	0.0000	0.9776
6	0.1567	0.0851	0.1643	0.5939
7 (Fuel Gas)	0.0780	0.0031	0.9132	0.0057
8	0.1734	0.1025	0.0057	0.7185
11	0.9392	0.0177	0.0308	0.0123
12	0.0000	0.1216	0.0000	0.8784
14 (Vent to Flare)	0.8194	0.0045	0.1643	0.0118
15 (DEE)	0.9643	0.0204	0.0028	0.0124
18 (Wastewater)	0.0000	0.0001	0.0000	0.9999
19	0.0000	0.1746	0.0000	0.8254

Table 9. Composition of different streams under optimized conditions.

	Energy Stream Name	Heat Flow (kJ/h)
Reaction Section	-	555120.8
Separation and Purification Section	q3	457494.8
	q4	49326.75
	q5	45746.74
	q6	4066.138
	q7	231699.4
	q8	206.8164
	q9	322055.5
	qc	55520.78
	qr	85013.41
	qc'	229255.3
	qr'	115,059
	Total	1,595,445
Total	-	2,150,566

Table 10. Energy consumption across various units in the reaction and separation/purification sections under optimized conditions.

of both DEE loss and energy consumption were set at minimum. But scenario 2 aims to set the value of energy consumption at the minimum value and DEE loss in range. The results of optimization of drum2 has been presented in Table 8. It is worthwhile noting that scenario 2 leads to liquid stream with zero flowrate that is not of interest. So, scenario 1 was selected as optimum condition.

Optimum condition

The results in Tables 9 and 10 are specifically related to the optimum operating conditions identified during the study. In other words, these results in both tables reflect the outcomes of operating the process under optimized conditions. As mentioned earlier, these conditions were carefully selected to maximize efficiency and sustainability, minimizing energy usage and material losses while achieving the desired DEE purity. According to Table 9, acceptable purity of DEE (96.43% in Stream 15) was achieved while minimizing ethylene, unreacted ethanol and water in the product stream. Additionally, the low DEE mol. fraction in waste streams (e.g., Stream 18 with 0% DEE) implies that the process is effectively separating DEE from others.

Table 10 details the energy consumption across various units in the reaction and separation/purification sections, while conducting the process at optimum conditions. According to this table, the energy required for the initial ethanol dehydration reaction is 555,120.8 kJ/h. In separation and purification section, energy is divided into multiple streams. Each of these streams represents the energy used in specific components like distillation columns, drums, heaters or coolers. The energy consumption in separation and purification section is 1,595,445 kJ/h. The total energy consumption for production process is 2,150,566 kJ/h. Accordingly, 1,499,754.87 kJ energy is needed for production of each kgmol DEE product with 96.43% purity.

Significance of the study

This research aims to improve the overall efficiency and sustainability of DEE production process. Further, the integration of process simulation with statistical modeling and optimization represents a robust and systematic approach that can be applied to other chemical processes. The scenario-based optimization strategy, where trade-offs between competing objectives (e.g., purity vs. energy consumption) are evaluated, can readily be applied to other processes seeking balanced performance.

The findings of this study are expected to contribute to the development of more energy-efficient and cost-effective DEE production processes. By identifying optimal operating conditions and strategies for the separation and purification section, this research aims to reduce energy consumption, minimize waste, and improve product quality. These improvements make this study interesting for both academic research and industrial applications.

Conclusion

This study optimized the separation and purification processes in diethyl ether (DEE) production by focusing on enhancing energy efficiency, minimizing material losses, and achieving high product purity. Through a systematic approach combining process simulation, statistical modeling, and optimization techniques, significant advancements were achieved in balancing technical and economic objectives. The optimization reduced DEE losses in fuel and vent streams that demonstrates improved efficiency in material recovery. Statistical models developed using response surface methodology (RSM) and central composite design (CCD) revealed critical non-linear relationships between operational parameters such as temperature and pressure that ensures reliable predictions of system performance with high accuracy. The study highlighted the trade-offs inherent in optimizing separation processes. The insights from scenario-based optimization emphasized the importance of integrating technical and economic considerations to achieve sustainable production. The findings align with global efforts to reduce the environmental footprint of industrial operations by enabling energy-efficient and cost-effective production methods. Since the proposed configuration is simulation-based, industrial trials or scale-up studies will be critical for translating theoretical energy savings and separation improvements into practical, commercially viable applications. Future work could explore the integration of energy generation from vent and fuel streams into current work. Further, future investigations should integrate catalyst recovery strategies to address operational and ecological challenges posed by homogeneous acid catalysts that ensures a more complete and sustainable DEE production process.

Data availability

"The datasets used and/or analysed during the current study available from the corresponding author on reasonable request."

Received: 17 February 2025; Accepted: 3 July 2025
Published online: 31 July 2025

References

1. Wu, L. et al. Process intensification of NaOH-catalyzed transesterification for biodiesel production by the use of bentonite and co-solvent (diethyl ether). *Fuel* **186**, 597–604 (2016).
2. Encinar, J. M., Pardal, A. & Sánchez, N. An improvement to the transesterification process by the use of co-solvents to produce biodiesel. *Fuel* **166**, 51–58 (2016).
3. Gargari, M. H. & Sadrameli, S. Investigating continuous biodiesel production from linseed oil in the presence of a Co-solvent and a heterogeneous based catalyst in a packed bed reactor. *Energy* **148**, 888–895 (2018).
4. Kumar, M. V., Babu, A. V. & Kumar, P. R. The impacts on combustion, performance and emissions of biodiesel by using additives in direct injection diesel engine. *Alexandria Eng. J.* **57**, 509–516 (2018).
5. Barik, D., Murugan, S., Samal, S. & Sivaram, N. Combined effect of compression ratio and diethyl ether (DEE) Port injection on performance and emission characteristics of a DI diesel engine fueled with upgraded biogas (UBG)-biodiesel dual fuel. *Fuel* **209**, 339–349 (2017).
6. Vignesh, R. et al. Adoptability assessment of HCDI and RCCI modes in plug-in parallel hybrid electric vehicles using sustainable fuels and model-based torque structure calibration strategies. *Results Eng.* **23**, 102859 (2024).
7. Charoensuppanimit, P., Chaiapha, B., Assabumrungrat, S. & Jongsomjit, B. Incorporation of diethyl ether production to existing bioethanol process: Techno-economic analysis. *J. Clean. Prod.* **327**, 129438 (2021).
8. Moghaddam, A. H. & Sargolzaei, J. Biofilm development on normal and modified surface in a hybrid SBR-based bioreactor. *J. Taiwan Inst. Chem. Eng.* **49**, 165–171 (2015).
9. Rahbar, A., Nekoomanesh-Haghighi, M., Bahri-Laleh, N. & Abedini, H. Effect of water on the supported Ziegler–Natta catalysts: optimization of the operating conditions by response surface methodology. *Catal. Lett.* **145**, 1186–1195 (2015).
10. Hedayati, A. & Moghaddam Investigation of natural gas dehydration process using triethylene glycol (TEG) based on statistical approach. *Chem. Pap.* **77**, 1433–1443 (2023).
11. Tashaouie, H. R., Gholikandi, G. B. & Hazrati, H. Artificial neural network modeling for predict performance of pressure filters in a water treatment plant. *Desalination Water Treat.* **39**, 192–198 (2012).
12. Sargolzaei, J. & Moghaddam, A. H. Predicting the yield of pomegranate oil from supercritical extraction using artificial neural networks and an adaptive-network-based fuzzy inference system. *Front. Chem. Sci. Eng.* **7**, 357–365 (2013).
13. Zhang, H., Juraskova, V. & Duarte, F. Modelling chemical processes in explicit solvents with machine learning potentials. *Nat. Commun.* **15**, 6114 (2024).

14. Savari, M., Moghaddam, A. H., Amiri, A., Shanbedi, M. & Ayub, M. N. B. Comprehensive heat transfer correlation for water/ethylene glycol-based graphene (nitrogen-doped graphene) nanofluids derived by artificial neural network (ANN) and adaptive neuro-fuzzy inference system (ANFIS). *Heat Mass Transf.* **53**, 3073–3083 (2017).
15. Durai, P., Lee, S. J., Lee, J. W., Pan, C. H. & Park, K. Iterative machine learning-based chemical similarity search to identify novel chemical inhibitors. *J. Cheminform.* **15**, 86 (2023).
16. Sadeq, A. M., Moghaddam, A. H., Sleiti, A. K. & Ahmed, S. F. Development of machine learning models for studying the premixed turbulent combustion of Gas-To-Liquids (GTL) fuel blends. *Korean J. Chem. Eng.* **41**, 479–494 (2024).
17. Kartal, F. & Özveren, U. Energy and exergy analysis of entrained bed gasifier/gt/kalina cycle model for CO2 co-gasification of waste tyre and Biochar. *Fuel* **331**, 125943 (2023).
18. Moghaddam, A. H., Esfandyari, M. & Sakhaeinia, H. Optimization of amine-based carbon capture: simulation and energy efficiency analysis of absorption section. *Results Eng.* **24**, 103574 (2024).
19. Zhou, X., Cai, Y. & Li, X. Process arrangement and multi-aspect study of a novel environmentally-friendly multigeneration plant relying on a geothermal-based plant combined with the Goswami cycle booted by Kalina and desalination cycles. *Energy* **299**, 131381 (2024).
20. Yi, C. Q. et al. Production of hydrogen using plastic waste via Aspen hysys simulation. *Sci. Rep.* **14**, 4934 (2024).
21. El Maghraby, M. A., El Moniem, N. A. & Abdelghany, A. Controlling hydrocarbon dew point and water dew point of natural gas using Aspen HYSYS. *J. Eng. Appl. Sci.* **69**, 66 (2022).
22. Moghaddam, A. H. Investigation and optimization of olefin purification in methanol-to-olefin process based on machine learning approach coupled with genetic algorithm. *Korean J. Chem. Eng.* **40**, 1168–1175 (2023).
23. Park, J., Yoon, S., Oh, S. Y., Kim, Y. & Kim, J. K. Improving energy efficiency for a low-temperature CO2 separation process in natural gas processing. *Energy* **214**, 118844 (2021).
24. Hedayati Moghaddam, A., Esfandyari, M., Jafari, D. & Sakhaeinia, H. Multi-factor optimization of bio-methanol production through gasification process via statistical methodology coupled with genetic algorithm. *Results Eng.* **20**, 101477 (2023).
25. Li, S., Inayat, M. & Järvinen, M. Steam gasification of polyethylene terephthalate (PET) with CaO in a bubbling fluidized bed gasifier for enriching H2 in Syngas with response surface methodology (RSM). *Appl. Energy*. **348**, 121536 (2023).
26. Ravald, H., Moghaddam, A. H., Jaikishan, S., Lavainne, M. & Wiedmer, S. K. Effect of liposome composition on β-blocker interactions studied by capillary electrokinetic chromatography. *J. Sep. Sci.* **46**, 2300414 (2023).
27. Thakur, A. & Dharmendra Electrocoagulation process modelling and optimization using RSM and ANN-GA for simultaneous removal of arsenic and fluoride. *Multiscale Multidisciplinary Model. Experiments Des.* **7**, 5899–5914 (2024).
28. Hedayati Moghaddam, A., Esfandyari, M. & Sakhaeinia, H. Investigation the effects of operational parameters and multi-factor optimization of Butene metathesis process via statistical approach. *Results Eng.* **23**, 102476 (2024).
29. Romelin, C., Zahedi, B. C. & Nusantara Comparative analysis of response surface methodology (RSM) and Taguchi method: optimization hydraulic Ram pump performance. *Oper. Res. Forum.* **5**, 85 (2024).
30. Hedayati Moghaddam, A. & Esfandyari, M. *Optimizing Diethyl Ether Production: Enhancing Efficiency and Sustainability Through Advanced Simulation and Statistical Analysis* (Energy Nexus, 2025).

Author contributions

Amin Hedayati Moghaddam: Writing – review & editing, Software, Resources, Methodology, Investigation. Morteza Esfandyari: Writing –review & editing, Methodology, Investigation, Conceptualization.

Declarations

Competing interests

The authors declare no competing interests.

Additional information

Correspondence and requests for materials should be addressed to A.H.M.

Reprints and permissions information is available at www.nature.com/reprints.

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.