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Research Article

Parametric Sensitivity Analysis in an Industrial Ethanol Distillation Column Using CHEMCAD-Based Modeling

Burak Dumlu*,[1], Taner Tekin*,[2]

[1]*Department of Chemical Engineering, Sugar Factory, Erzurum, Türkiye*
[2]*Department of Chemical Engineering, Atatürk University, Erzurum, Türkiye*

Keywords

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NRTL,
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Reboiler Duty,
Product column.

Abstract

In industrial ethanol production, distillation and rectification columns are among the most energy-intensive process units. In this study, the product column of an industrial-scale ethanol production plant was modeled using CHEMCAD to investigate the effects of key operating parameters on column performance. The NRTL thermodynamic model was used to represent the non-ideal ethanol–water system. The modeled column consisted of 60 theoretical stages, and the feed composition was defined by liquid volume fractions of 0.91667 water, 0.08312 ethanol, and 0.00021 methanol. A one-factor-at-a-time (OFAT) parametric sensitivity analysis was performed by varying the reflux ratio, feed tray position, and feed temperature while maintaining the remaining operating conditions at their reference values. Distillate ethanol concentration, bottoms ethanol concentration, ethanol mass distribution, and reboiler duty was evaluated as performance indicators. Increasing the reflux ratio improved distillate ethanol concentration and reduced ethanol losses in the bottoms stream, but resulted in higher energy consumption. Moving the feed location upward improved ethanol recovery, with only marginal performance changes beyond tray 21. Increasing the feed temperature reduced reboiler duty. Considering the trade-offs among product purity, ethanol recovery, and energy consumption, a reflux ratio of R/D = 6, feed tray 21, and a feed temperature of 55 °C were identified as the most favorable operating conditions within the investigated ranges. These results provide an engineering basis for evaluating operating parameter effects rather than representing a global optimization of the column.

1. Introduction

Industrial ethanol production begins with the fermentation of sugar or starch-based raw materials. During the fermentation stage, microorganisms convert sugars into ethanol and carbon dioxide; the fermentation output is a low-concentration ethanol-water mixture. This mixture is fed into multi-stage distillation and rectification columns for the production of ethanol with a purity of approximately 96% according to industrial standards. In the distillation and rectification steps, ethanol is enriched in the overhead product stream by taking advantage of the volatility differences between the components, while water and heavy components are removed from the bottom products [1].

When higher purity is required in fuel or chemical process applications, ethanol concentration can be increased to 99.8% using dehydration methods such as molecular sieves. However, distillation and rectification units account for a significant portion of the plant's total energy costs due to high steam consumption. Therefore, the optimization of parameters such as reflux ratio, feed tray position, column pressure, number of trays, feed conditions, and heat integration is critical for both reducing energy consumption and maintaining product quality [2].

Within the scope of this study, the product column of an industrial ethanol production plant was modeled using ChemCAD software, and the effects of column operating parameters on quality and energy consumption were evaluated [3]. Specifically, the reflux ratio, feed tray position, and feed temperature were systematically varied, and their individual effects on distillate ethanol concentration, bottoms ethanol loss, and reboiler duty were evaluated to identify the most favorable operating conditions within the investigated parameter ranges.

2. Materials and Methods

2.1. Process Description

This study examines the product column within a multi-stage distillation system that purifies the aqueous alcohol mixture from the fermentation effluent. The product column aims to produce high-purity ethanol in the overhead product that meets industrial standards, while minimizing ethanol losses in the bottom product stream.

2.2. ChemCAD Model and Thermodynamic Package Selection

The product column was modeled using ChemCAD software, and the diagram is shown in Figure 1. The NRTL (Non-Random Two-Liquid) model, which is widely used for ethanol–water systems as a thermodynamic package and is based on activity coefficients, was selected. This selection was made to more accurately represent the non-ideal liquid phase behavior in the ethanol–water system [3].

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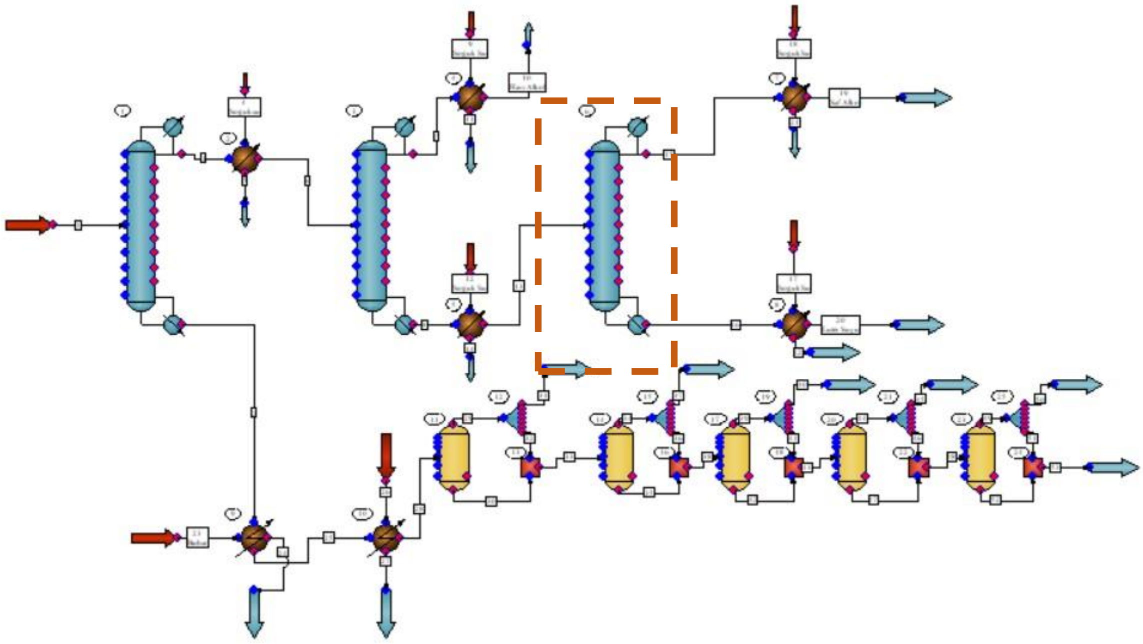

Figure 1. ChemCAD flow diagram of the ethanol distillation system

2.3. Column Configuration and Feed Definition

The industrial ethanol product column was modeled in CHEMCAD 8.0 using the built-in equilibrium-stage tray column model under steady-state conditions. The column consisted of 60 theoretical stages with a total condenser configuration. Atmospheric operating conditions were assumed throughout the simulation, and both the feed stream and condenser pressure were specified as 1.013 bar.

The reference column configuration was established based on the product distillation column of the Erzurum Ethanol Plant, which was originally commissioned in 1986 and remained in operation until 2004. Although the facility is currently undergoing modernization and no recent industrial production data are available for validation, the geometric configuration of the existing product column, including the 60-stage arrangement, was adopted as the baseline configuration for the present simulation study. Therefore, the selected number of stages represents an industrial reference rather than an arbitrary theoretical design.

The condenser operating specification was defined by the reflux ratio (R/D), whereas the reboiler operating specification was defined by the bottom product mass flow rate. In the reference simulation, the reflux ratio was fixed at 6 and the bottom product mass flow rate was specified as 14,225 kg/h. The reference feed stage was tray 21.

The feed stream entered the column at 50 °C and 1.013 bar with a total volumetric flow rate of 15.5787 std m^3/h. The liquid volume fractions of the feed were specified as 0.91667 water, 0.08312 ethanol, and 0.00021 methanol, representing the composition of the stream entering the product column after the preceding separation stages.

The simulations were performed under steady-state conditions using the equilibrium-stage model available in CHEMCAD 8.0. During the parametric sensitivity analysis, only one operating parameter was varied at a time while all remaining operating conditions were maintained at their reference values. The investigated parameters included reflux ratio, feed tray location, and feed temperature.

Unless otherwise stated, all simulations were carried out using the same column configuration and operating specifications to ensure direct comparison between the investigated cases.

2.4. Parametric Sensitivity Analysis and Performance Criteria

A one-factor-at-a-time (OFAT) parametric sensitivity analysis was performed to evaluate the influence of the main operating parameters on column performance. In each simulation, only one operating parameter was varied while all remaining operating conditions were kept constant. This approach allowed the individual effect of each parameter to be evaluated independently and enabled direct comparison of their influence on product quality and energy consumption.

The investigated operating parameters were as follows:

* Reflux ratio (R/D)

* Feed tray position

* Feed temperature

The following performance indicators were monitored:

* Distillate ethanol concentration (Distillate Ethanol Volume Fraction)

* Bottom product ethanol loss (Bottom Ethanol Volume Fraction)

* Reboiler Duty (MW)

These performance indicators were selected because they represent the primary engineering objectives of an industrial ethanol product column: maximizing ethanol purity, minimizing ethanol loss in the bottom product, and reducing energy consumption. The results obtained from each simulation were compared collectively to identify the most appropriate operating conditions within the investigated parameter ranges.

2.5. Consistency-Based Model Evaluation

Since direct historical operating data from the Erzurum ethanol plant were not available, the simulation model was evaluated using internal consistency checks and literature-based engineering expectations. First, the simulated distillate ethanol concentrations were compared with the typical azeotropic ethanol purity range obtained in conventional ethanol–water distillation systems. The predicted distillate ethanol concentrations, which ranged approximately between 94.3 and 95.7 vol%, were consistent with the expected concentration range for atmospheric ethanol rectification prior to dehydration.

Second, mass balance consistency was assessed by monitoring both distillate ethanol mass flow rate and bottom ethanol mass flow rate in addition to volumetric ethanol fractions. The results showed that increases in distillate ethanol recovery were accompanied by corresponding decreases in bottom ethanol losses, indicating physically consistent component distribution within the column.

Third, the energy behavior of the model was checked against established distillation principles. Increasing the reflux ratio increased column reboiler duty, while increasing the feed temperature reduced the reboiler heat requirement due to the higher enthalpy of the feed stream. These trends are consistent with conventional distillation theory and confirm that the simulated responses follow expected engineering behavior.

These consistency checks do not constitute external validation of the simulation model, since direct plant-scale experimental data were unavailable. Nevertheless, they demonstrate that the simulated results are consistent with literature-based expectations, component mass-balance behavior, and established distillation principles, supporting the use of the model for comparative parametric sensitivity analysis within the investigated operating range.

3. Findings and Discussion

3.1. Effect of Reflux Ratio on Column Performance

The reflux ratio was varied between 4 and 8, and the distillate ethanol concentration, bottoms ethanol concentration, and Reboiler Duty were evaluated, as presented in Table 1.

Table 1. Effect of Reflux Ratio on Column Performance

Reflux ratio	Distilled Ethanol (Vol%)	Bottom Ethanol (Vol%)	Reboiler Duty (MW)	Distillate Ethanol Mass kg/h	Bottom Ethanol Mass kg/h
4	0.94304	0.00163	2.279	1012.754	18.434
5	0.94571	0.00131	2.547	1016.322	14.866
6	0.9475	0.0011	2.826	1018.707	12.481
7	0.94877	0.00095	3.105	1020.421	10.767
8	0.94973	0.00084	3.384	1021.711	9.477

A graph was created from these values and is shown in Figure 2.

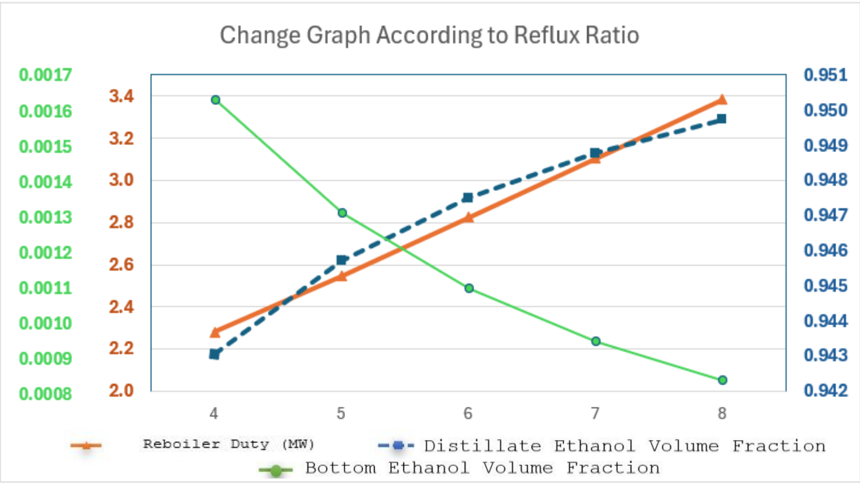

Figure 2. Effect of Reflux Ratio on Distillate Ethanol Concentration, Bottoms Ethanol Concentration, and Column Reboiler Duty

Increasing the reflux ratio from 4 to 8 increased the distillate ethanol volume fraction from 0.94304 to 0.94973 (corresponding to 94.304 to 94.973 vol%), while the bottom ethanol volume fraction decreased from 0.00163 to 0.00084 (corresponding to 0.163 to 0.084 vol%). This indicates that increasing the reflux ratio improves ethanol enrichment in the distillate while reducing ethanol losses in the bottom product [4].

However, increasing the reflux ratio resulted in a substantial increase in reboiler duty. When the reflux ratio was 4, energy consumption was 2.279 MW, but when the reflux ratio was increased to 8, energy consumption rose to 3.384 MW. It was observed that increasing the reflux ratio beyond 6 resulted in marginal improvements in distillate ethanol purity, while energy consumption continued to increase. Therefore, considering the trade-off between ethanol purity and energy consumption, a reflux ratio of R/D = 6 was selected as the most favorable operating condition within the investigated range.

At a reflux ratio of R/D = 6, the simulated methanol concentration in the distillate was 0.00126 as a liquid volume fraction, corresponding to 0.126 vol%. This value is below the maximum methanol limit of 0.5 vol% specified for fuel ethanol [6].

3.2. Effect of Feed Tray Position on Column Performance

The feed tray position was varied from tray 10 to tray 23, and the distillate ethanol concentration, bottoms ethanol concentration, and reboiler duty were evaluated, as presented in Table 2.

Table 2. Effect of Feed Tray Position on Column Performance

Feed Tray	Distilled Ethanol Volume Fraction	Bottom Ethanol Volume Fraction	Reboiler Duty (MW)	Distillate Ethanol Mass kg/h	Bottom Ethanol Mass kg/h
10	0.9399	0.00199	2.849	1008.604	22.5834
11	0.94292	0.00164	2.849	1012.625	18.5628
12	0.94541	0.00135	2.837	1015.943	15.245
13	0.94749	0.0011	2.826	1018.711	12.4777
14	0.94925	0.00089	2.826	1021.05	10.1373
15	0.95075	0.00072	2.814	1023.053	8.1348
16	0.95206	0.00056	2.814	1024.795	6.3924
17	0.95319	0.00043	2.802	1026.305	4.883
18	0.95419	0.00031	2.802	1027.64	3.5476
19	0.95507	0.00021	2.802	1028.821	2.3672
20	0.95586	0.0001	2.791	1029.879	1.3093
21	0.95656	0.00003	2.791	1030.813	0.3754
22	0.95674	<numerical tolerance	2.791	1031.183	0.0047
23	0.95662	<numerical tolerance	2.791	1031.188	<numerical tolerance

Values reported as "< numerical tolerance" are below the numerical resolution limit of the simulation output and should not be interpreted as absolute zero.

A graph was created from these values and is shown in Figure 3.

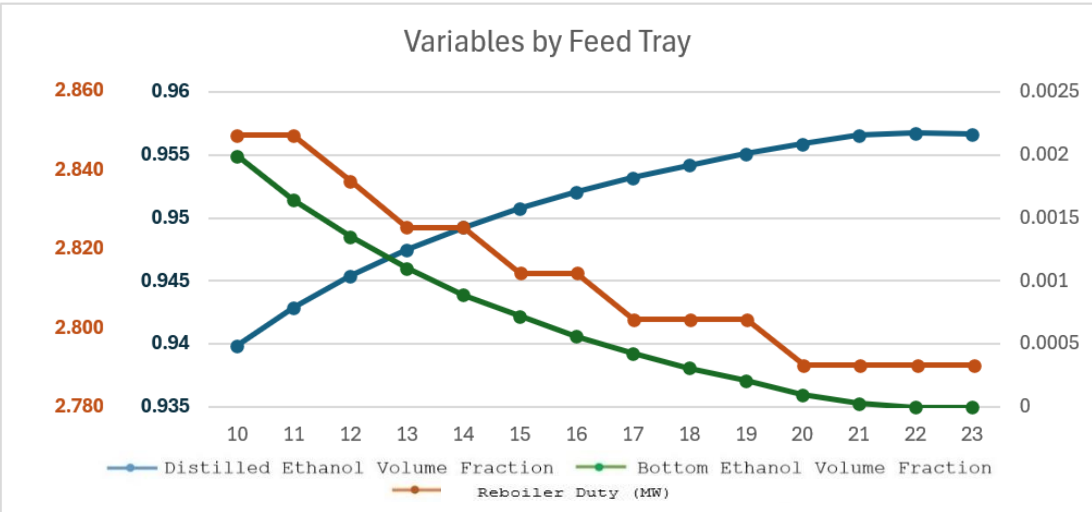

Figure 3. Effect of Feed Tray Position on Distillate Ethanol Concentration, Bottoms Ethanol Concentration, and Column Reboiler Duty

As the feed tray position was shifted upward from tray 10 to tray 23, the ethanol concentration in the distillate gradually increased, while ethanol loss in the bottom product decreased substantially. Beginning at tray 21, the calculated bottom ethanol loss approached the numerical resolution limit of the simulation, and no meaningful additional reduction was observed at higher tray positions. Likewise, energy consumption changed only marginally beyond trays 20–21, indicating that further upward movement of the feed tray produced negligible performance improvement [5].

Based on the combined evaluation of distillate ethanol concentration, bottoms ethanol concentration, and energy consumption, tray 21 was selected as the most appropriate feed location among the investigated cases. Although trays 22 and 23 resulted in slightly lower calculated bottoms ethanol levels, these values approached the numerical tolerance of the simulation and provided no meaningful additional improvement in energy consumption or distillate ethanol concentration. From an operational perspective, industrial columns may experience shifts in vapor–liquid traffic due to variations in feed flow rate and operating conditions. Such shifts may alter the internal vapor–liquid balance and potentially increase ethanol losses through the cooler vents. Therefore, tray 21 was preferred as a practical operating point within the investigated range, while avoiding reliance on results approaching the numerical tolerance of the simulation [5].

The increase in distillate ethanol volume fraction between trays 21 and 23 was only 0.00006, whereas bottom ethanol loss and reboiler duty remained essentially unchanged. These results indicate that additional increases in feed tray position provide diminishing performance improvements.

3.3. Effect of Feed Temperature on Column Performance

The feed temperature was varied from 40 to 60 °C, and its effects on distillate ethanol concentration and reboiler duty were evaluated, as presented in Table 3.

Table 3. Effect of Feed Temperature on Column Performance

Feed Temperature	Distilled Ethanol Volume Fraction	Bottom Ethanol Volume Fraction	Reboiler Duty (MW)	Distillate Ethanol Mass kg/h	Bottom Ethanol Mass kg/h
40	0.9566	0.00003	2.965	1030.866	0.3228
45	0.95658	0.00003	2.884	1030.844	0.3438
50	0.95656	0.00003	2.791	1030.816	0.3722
55	0.95654	0.00003	2.709	1030.78	0.4081
60	0.95651	0.00003	2.616	1030.756	0.4321

In the simulation results, changes in feed temperature did not significantly affect the loss of the bottoms product ethanol. Therefore, the bottoms product loss was not included in the graph.

A graph was created from these values and is shown in Figure 4.

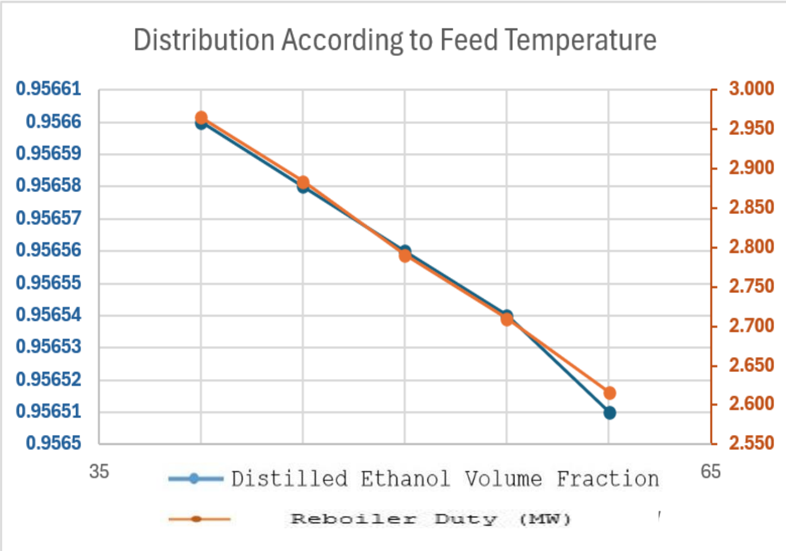

Figure 4. Effect of Feed Temperature on Distillate Ethanol Concentration and Column Reboiler Duty

Simulation results indicate that increasing the feed temperature from 40°C to 60°C produced only a negligible reduction in distillate ethanol concentration, whereas reboiler duty decreased steadily throughout the investigated temperature range. The higher feed temperature increased the enthalpy of the incoming stream, thereby reducing the reboiler heat duty and lowering the overall energy requirement of the distillation column.

The practical heat-recovery configuration considered in this study supports feed preheating up to the targeted temperature of 55 °C. The 60 °C case was included as a theoretical sensitivity scenario to evaluate the model response beyond this practical operating condition; therefore, it should not be interpreted as an equally feasible industrial alternative without additional external heating or further verification of the available waste-heat capacity. This assumption reflects the current modernization strategy planned for the Erzurum Ethanol Plant and represents the intended industrial operating configuration rather than an arbitrary theoretical assumption.

Although the minimum energy consumption was obtained at 60°C, the additional reduction in energy consumption beyond 55°C was limited. Between 55°C and 60°C, energy consumption decreased by only 0.093 MW (approximately 3.4%), while the distillate ethanol concentration showed a slight decrease from 0.95654 to 0.95651 in volume fraction (corresponding to 95.654 to 95.651 vol%). These results indicate diminishing returns in energy savings at temperatures above 55°C, as relatively small energy savings are accompanied by a gradual reduction in product purity.

Based on the trade-off between energy consumption and ethanol purity, a feed temperature of 55 °C was considered the preferred operating condition within the investigated range. This selection represents an engineering trade-off among the investigated cases rather than a uniquely determined optimum.

4. Conclusion and Evaluation

Within the scope of this study, the product column used in industrial ethanol production was modeled using CHEMCAD software, and the effects of the main operating parameters on column performance were investigated through a one-factor-at-a-time (OFAT) parametric sensitivity analysis. The investigated parameters included reflux ratio, feed tray location, and feed temperature. The evaluation was based on three engineering performance indicators: distillate ethanol concentration, bottom ethanol loss, and reboiler duty.

The simulation results showed that increasing the reflux ratio improved distillate ethanol purity while simultaneously increasing energy consumption. Considering the combined evaluation of product purity and energy demand, a reflux ratio (R/D) of 6 was identified as the most favorable operating condition within the investigated range.

The feed tray analysis demonstrated that moving the feed location upward increased distillate ethanol concentration and reduced ethanol loss in the bottom product. However, the improvements became negligible beyond tray 21, while energy consumption remained essentially unchanged. Therefore, tray 21 was selected as the most appropriate feed location among the investigated cases.

Increasing the feed temperature reduced the energy requirement of the distillation column due to the higher thermal content of the incoming feed stream. Although a feed temperature of 60 °C provided slightly lower energy consumption, the improvement in ethanol purity became negligible beyond 55 °C. Based on the combined evaluation of product purity and energy consumption, a feed temperature of 55 °C was selected as the preferred operating condition.

Within the investigated operating ranges, the combination of a reflux ratio of 6, a feed tray location of 21, and a feed temperature of 55 °C provided the most favorable balance between distillate ethanol purity, bottom ethanol loss, and energy consumption. These findings are applicable only to the investigated simulation model and parameter ranges and should be interpreted as the results of a parametric sensitivity analysis rather than a global optimization study.

5. Future Work

The parametric sensitivity analyses carried out within the scope of this study were performed using a one-factor-at-a-time (OFAT) approach on the product column. More comprehensive analyses are planned in future studies under the following headings:

Multivariate optimization studies (multi-objective optimization)

Similar analyses for other distillation columns in the system outside the product column

Energy cost and economic benefit analysis (annual savings based on steam cost)

Industrial application and field validation: testing the identified operating conditions at the pilot/field scale at the Erzurum ethanol plant.

Author Contributions

B.D.: Conceptualization, Methodology, Software, Formal Analysis, Investigation, Data Curation, Visualization, Writing – Original Draft. T.T.: Conceptualization, Methodology, Supervision, Validation, Writing – Review & Editing.

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Data Availability Statement

The data presented in this study are available from the corresponding author upon reasonable request.

Conflict of Interest Statement

The authors declare that there is no conflict of interest. They have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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