Lecture Notes in Networks and Systems 2170

Rafik Aziz Aliev ·
Nodirbek Rustambekovich Yusupbekov ·
Janusz Kacprzyk · Witold Pedrycz ·
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Preface

This volume presents an edited selection of the presentations from the 13th World Conference on Intelligent Systems for Industrial Automation, WCIS-2024, which was held in Tashkent, Uzbekistan, 24–25 October 2024. WCIS-2024 is held as a meeting for the communication of research on application of fuzzy logic, neural networks and AI for solving control, decision-making, analysis, monitoring and other problems in industry and related fields. The conference provided an opportunity to present and discuss state-of-the-art research in this expanding domain.

This volume will be a useful guide for academics, practitioners, and graduates in the scope of intelligent industrial systems. It will allow for increasing interest in the development and applying methods of intelligent control and decision-making in various industry applications.

October 2024

Rafik Aziz Aliev
Nodirbek Rustambekovich Yusupbekov
Chairmen of WCIS-2024

Modeling of the Digital Twin for Wind Turbines 199
Ogtay Rasulzade

Assessment of Performance Risks in Digital Advertising Platforms Using Fuzzy Logic 206
Rahib Imamguluyev, Ramiz Alekperov, Aliyev Vusal, and Niyar Umarova

Construction of a Production Function for the Transport Sector Under Z-Number-Based Information 213
V. J. Akhundov

Graph Theory Matrix Approach of Multi-Criteria Decision Analysis for Evaluation and Ranking of Cars 221
Aida Aliyeva and Hasan Temizkan

Digitalization and Artificial Intelligence in Public Administration: Opportunities, Challenges and Strategic Approaches 230
Murat Tüzünkan

Rank Reversal-Free Approach to Digital Marketing Technologies Selection 239
Gunay E. Imanova and Gunel Imanova

Kinematic Modeling of Lower Limb Rehabilitation Exoskeleton Robots Using MATLAB 248
Umidjon Takabaev, Zafar Juraev, Javlonbek Rakhmatillaev, and Nodirbek Kimsanboev

Application of Fuzzy Logic–Based Decision Support System for Diagnosis Under Uncertainty 255
Charos Khidirova, Muhabbat Sharapova, Shakhnoza Sadikova, and Nozima Jabborova

Modeling and Analysis of the Process of Fractional Separation in a Rectification Column 264
Sh. Doliev, S. Farkhodov, X. Yusupov, and R. Toshtemirov

Mathematical Modeling of Dynamic Modes of Rectification Process under Uncertainty Conditions 271
Yusuf Shodiyevich Avazov, Umidjon Abdimajitovich Ruziev, and Kamola Rustamovna Abdullaeva

Vapor-Phase Synthesis of Vinyl Acetate from Acetylene Over Bentonite-Supported Zn–cd Acetate Catalysts: Structure–Activity Relationships and Reaction Mechanism 277
S. M. Turabjanov, Kh. I. Kadirov, O. O. Zaripov, and O. R. Maksudov

Modeling and Analysis of the Process of Fractional Separation in a Rectification Column

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Abstract. Today, oil, gas, and chemical industries, rectification columns are considered one of the most critical pieces of industrial equipment in the process of separating liquids into fractions. Therefore, this article presents a simulation of the separation of benzene and toluene into fractions within a rectification column using Aspen Plus software, along with an analysis of this process. This modeling approach enhances the ability to study and optimize the technological process by conducting experiments based on a modern software platform, rather than performing real-world physical and practical experiments. This research was conducted to optimize the fractionation process of the liquid mixture and increase the purity of the separated components, thereby achieving a higher level of separation efficiency. The modeling process carried out in the study improved the ability to control variables such as temperature, pressure, and reflux ratio. The optimal control of these parameters made it possible to improve the quality of the distillate and bottom product emerging from the rectification column. The results determined that it is possible to separate benzene at 90% purity and toluene at 99% purity in the rectification column. By utilizing such modern modeling methods and software, it is possible to obtain suggestions and recommendations for increasing efficiency and optimizing the substance fractionation process.

Keywords: Rectification columns · Fractional distillation · Modeling · Aspen plus · Separation efficiency · Benzene · Toluene

1 Introduction

Today, in industries such as oil, gas, and chemicals, the separation of raw materials into fractions - that is, their constituent components - is a critical part of the substance processing cycle. However, this process faces several challenges. Solving these issues is particularly urgent given the rising demand for energy. Examples of these problems include high energy consumption during fractionation and the low quality (purity) of the separated components. In the fractionation process, the specific point at which the mixture enters a single rectification column - meaning the tray where it is introduced - significantly affects both the quality of the separated component and the amount of energy consumed during the separation. Furthermore, the efficiency of the fractionation process

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depends on several parameters, such as temperature, pressure, and reflux ratio. In this context, optimally managing these variable parameters is crucial; however, conducting practical and physical experiments to control them has been observed to entail certain difficulties and costs. In such cases, it is necessary to use a suite of technical systems (such as Aspen Plus) to achieve a high-quality separation of the distillate and bottom product in a rectification column unit [1]. In recent years, virtual modeling methods have become a modern, innovative tool for optimizing processes across various industries, emerging as a safe, cost-effective, and flexible platform for studying and improving complex processes and systems. By utilizing such software, it is possible to obtain significant results and develop recommendations for the optimal control of the rectification process [2].

Today, several modern software programs are available for modeling technological processes, one of which is Aspen Plus. Sources [3] note that this program offers a range of capabilities for developing simulations, designs, and optimization proposals corresponding to real-world industrial processes. Specifically, these capabilities include observing changes in thermodynamic and mass transfer processes, as well as obtaining detailed data and results on energy consumption, balances, and several other important indicators. The results of studies conducted by numerous researchers show that this program enables the modeling and simulation of a rectification column under various conditions. Integrating Aspen Plus with other modeling software further expands the possibilities for simulating and modeling complex chemical processes. Moreover, this approach not only facilitates a more in-depth study of the technological process but also promotes the optimization of system parameter control. Additionally, using Aspen Plus, it is possible to obtain results on how to improve the separation quality of liquid mixtures in rectification units, select the optimal number of trays, and achieve energy efficiency.. In their research on the rectification process, researchers can simulate various operating conditions, identify the factors influencing the purity of the separated components, and quickly evaluate them. They can also conduct experiments through the software based on various scenarios.

2 Methodology

The objective of this research is to separate a mixture into its constituent fractions using a rectification column, specifically focusing on how to obtain high-purity benzene and toluene fractions. Additionally, it shows that energy efficiency can be increased by analyzing the heat load during the mixture separation process. This study presents data on the effective management of the rectification process, utilizing a virtual modeling approach. By adjusting technological parameters such as temperature, pressure, and reflux ratio, the process enables the high-quality (pure) separation of a mixture into distillate and bottoms within a rectification column.

Before modeling the fractionation process in Aspen Plus, we first establish the material balances for the liquid mixture. Subsequently, we perform the virtual modeling by executing a series of steps within the software. During the modeling process, the names of the components in the mixture are entered, a thermodynamic method is selected, and the technological scheme of the separation process is constructed in the simulation environment. Additionally, the required parameter values for the separation process are input

into the program, the necessary number of experiments are conducted, and the results are obtained. The obtained results are then analyzed. In our research, we will investigate how to determine the optimal feed tray in the upper section of the rectification column to achieve the highest separation efficiency for a benzene (mole fraction 0.32) - toluene (mole fraction 0.68) mixture. The mixture is fed to the rectification column at a flow rate of 8000 kg/h and a pressure of 1 bar. Based on the boiling point of benzene, the mixture temperature is 82 °C. The total number of trays in the column was assumed to be 25 during the initial experiments [4]. The values required for the virtual modeling were determined using the material balance equations [5] presented below, which also allows for the determination of the minimum and operating reflux ratios necessary for the modeling process. The values presented below were determined as they are essential for the modeling process.

Distillate:

$$G_D = G_F \cdot \frac{X_f - X_w}{X_d - X_w} = 8000 \frac{32 - 1.8}{96 - 1.8} = 2564.7 \text{ kg/hr} \tag{1}$$

Bottom:

$$G_w = G_f - G_D = 8000 - 2564.7 = 5435.3 \text{kg/hr} \tag{2}$$

Rectification column input feed:

$$X_F = \frac{\frac{X_f}{M_{ben}}}{\frac{X_f}{M_{ben}} + \frac{100 - X_f}{M_{tol}}} = \frac{\frac{32}{79}}{\frac{32}{79} + \frac{100-32}{92}} = 0,354 \tag{3}$$

The molar fraction of distillate

$$X_D = \frac{\frac{X_d}{M_{ben}}}{\frac{X_d}{M_{ben}} + \frac{100 - X_d}{M_{tol}}} = \frac{\frac{96}{79}}{\frac{96}{79} + \frac{100-96}{92}} = 0,965 \tag{4}$$

The molar fraction of the bottom:

$$X_W = \frac{\frac{X_w}{M_{ben}}}{\frac{X_w}{M_{ben}} + \frac{100 - X_w}{M_{tol}}} = \frac{\frac{1.8}{79}}{\frac{1.8}{79} + \frac{100-1.8}{92}} = 0,0209 \tag{5}$$

Relative molar flow rate of rectification column input feed:

$$F = \frac{X_{d-X_w}}{X_F - X_w} = \frac{0,965 - 0,0209}{0,354 - 0,0209} = 2.834 \tag{6}$$

Minimum reflux ratios number:

$$R_{min} = \frac{X_{D-Y^*_F}}{Y^*_F - X_F} = \frac{0,965 - 0,57}{0,57 - 0,354} = 1.828 \tag{7}$$

Working reflux ratios number:

$$R = 1,3 \times R_{min} + 0,3 = 1,3 \times 1.828 + 0,3 = 2.67 \tag{8}$$

The names of the components in the mixture being fed into the rectification column unit are registered as BENZENE and TOLUENE in the Component ID section of the Aspen Plus Properties workspace [6].

One of the most widely used thermodynamic empirical methods for mixture separation processes in Aspen Plus is the UNIFAC (Universal Quasi-Chemical Functional Group Activity Coefficients) method. This is considered a reliable and effective method for predicting the activity coefficients of the liquid phase in non-electrolyte mixtures at low to moderate pressures and at temperatures from 300 to 425 K [7, 8].

Furthermore, it is mentioned in [9] that this method can also be used in research to model mixtures containing water, hydrocarbons, alcohols, chlorides, nitriles, ketones, amines, and other organic liquids within this temperature range. The UNIFAC method primarily separates molecules by utilizing their functional group cross-sections. In this case, each existing molecule consists of a combination of different groups, and the interactions between these groups are used to determine phase equilibrium. The activity coefficient, which accounts for molecular interactions, is calculated by the UNIFAC method. This coefficient represents the difference between the ideal and real states of the components within the mixture. If we focus on the two main effects of this method, they are as follows:

1. Combinatorial effect: Related to the size and shape of the molecules.

2. Interactions arising from polar and dispersion forces: Calculated based on the chemical forces between molecules. Because the UNIFAC method models molecules based on their functional groups, it allows for faster results during the process of separating a mixture into fractions [10].

The molar masses and boiling points of the components in the mixture were determined using the Review command, located in the Properties section of the Aspen Plus software, and are presented in Table 1.

Table 1. The molar mass and boiling point of benzene and toluene

№	Parameter names	Benzene	Toluene
1	MW	78,1136	92,1405
2	TB	80,09 °C	110,63 °C

In designing the process flowsheet, a RadFrac column was selected for rectification. The technological scheme for the process of separating the mixture into fractions was constructed in the Simulation environment of the Aspen Plus software.

The process of configuring the RadFrac column parameters begins with the total number of trays in the column; the program is set to a total of 25 trays. Based on the complete vaporization of the mixture within the column, the Total condenser command is selected. The mixture inside the column consists of vapor and liquid phases. This is because at least one of the components in the mixture is at a temperature above its boiling point. The total amount of benzene in the mixture is considered the distillate leaving the top of the column. Toluene, in turn, is equal to the amount of bottoms residue

separating from the bottom of the column. We enter the reflux ratio based on the results of the above calculations.

3 Discussion

By changing the feed point of the mixture to the upper plates of the column, we obtain the following results Tables 2 and 3.

Table 2. The percentage of benzene in the inlet fraction at a temperature of 82 °C at specified trays.

Benzene			
The inlet point of the incoming product	Temperature (°C)	Fraction percent	Heat duty (Watt)
5	82	0,904544679	−1029341,653
10	82	0,904725058	−1029359,476
15	82	0,897158034	−1029361,138
20	82	0,857224426	−1029123,332
Difference		0,047320252	−218,3206851

Experimental results show that the amount of heat consumption can be reduced by identifying the optimal feed point for the mixture among the column's trays. When the mixture is fed into the column at the 15^{th} tray, it is possible to reduce heat consumption by 218 watts per hour and increase separation efficiency by up to 4.73% (Table 3).

Table 3. The percentage of toluene in the inlet fraction at a temperature of 82 °C at specified trays.

Toluene			
The inlet point of the incoming product	Temperature (°C)	Fraction percent	Heat duty (Watt)
5	82	0,99895734	−1029341,653
10	82	0,999071259	−1029359,476
15	82	0,994293307	−1029361,138
20	82	0,969400164	−1029123,332
Difference		0,029557176	−218,3206851

The experimental results show that heat consumption can be reduced by finding the optimal feed point for the mixture among the column trays. When the mixture is fed

into the column at the 15th tray, it becomes possible to reduce heat consumption by 218 watts per hour and alter the separation efficiency by up to 2.95%. Analyzing the research results above, it was determined that the highest separation efficiency can be achieved if the mixture is fed into the column at the 12th tray. The results obtained are reflected in the table below (Table 4).

Table 4. Efficiency of benzene and toluene separation (in percent) when the mixture is fed to the 12th tray of the rectification column.

Mole Fractions		(Benzene)	(Feed)	(Toluene)
Benzene	%	0,096817511	0,32	0,001904261
Toluene	%	0,096817511	0,68	0,998095739

4 Conclusion

In conclusion, when a mixture is fed into a rectification column for fractionation, the correct and optimal selection of the feed point significantly impacts the quality and efficiency of the separation. This selection also allows for the modification of the process's heat load requirements. In turn, adjusting these heat load requirements alters the amount of energy consumed during the fractionation process. Modeling such operations using modern software presents a contemporary solution for optimizing technological processes in industry.

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