Journal of Chemical Engineering Research Updates, 2025, 69-83

Published by Avanti Publishers

Journal of Chemical Engineering Research Updates

ISSN (online): 2409-983X

Comparative Analysis and Optimization of Separation Technique of Carboxylic Acid-Water Mixture Using Aspen Plus

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ARTICLE INFO

Article Type: Research Article

Academic Editor: Cai Yitao

Keywords:
Water
Acetic acid
Extractive distillation
Azeotropic distillation

Timeline:
Received: May 29, 2025
Accepted: September 25, 2025
Published: November 03, 2025

Citation: Prabhakar A, Raghav S, Samridhi, Mishra Y. Comparative analysis and optimization of separation technique of carboxylic acid-water mixture using aspen plus. J Chem Eng Res Updates. 2025; 12: 69-83.

DOI: https://doi.org/10.15377/2409-983X.2025.12.5

ABSTRACT

Acetic acid (ethanoic acid) is widely employed as a food preservative, a versatile solvent, and as an intermediate in the synthesis of various industrial chemicals. Recent studies have emphasized process intensification strategies for its separation. Conventional distillation, though straightforward, requires a large number of trays and significant energy input. In contrast, azeotropic and extractive distillation offer improved efficiency with fewer stages and lower energy demand. This study investigates the separation of acetic acid–water mixtures using azeotropic and extractive distillation. Among the azeotropic agents, isobutyl acetate demonstrated lower energy consumption and reduced total annual cost (TAC) compared to vinyl acetate, while achieving high product purity (98.6% acetic acid and 99% water). For extractive distillation, methyl tert-butyl ether (MTBE) exhibited superior performance, yielding 99% purity for both acetic acid and water with minimum energy requirement and solvent usage, outperforming ethyl acetate, which achieved 98.2% acetic acid and 99% water. In comparison, conventional distillation provided only 92.1% acetic acid and 86.4% water. Overall, extractive distillation with MTBE proved to be the most efficient and cost-effective option for acetic acid purification.

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1. Introduction

Acetic acid, also known as ethanoic acid, is widely utilized in the process industries for a variety of purposes in wide range of industrial applications as a solvent, including the synthesis of polyvinyl acetate, cellulose acetate, and polyethylene terephthalate [1]. There are numerous industries that use these chemical compounds, including textile, automotive, food, packaging, paint, and construction [2]. Vinegar's main ingredient, acetic acid, has use in science, medicine, and food [3-6]. Chemical industries largely dependent on ethanoic acid as a basic organic chemical material [7], and it comes under the category of 20 important intermediates in the chemical industries [8, 9], also it is mostly utilized in the production of various polymers, adhesives, paints and acetic anhydride [10]. The combinations of water and acetic acid are used in the synthesis of a variety of intermediates such as vinyl acetate, and other anhydrides [9-11]. Acetic acid is becoming more and more in demand due to these industries' growing needs. From 6 million tons in 2014 to 12.1 million tonnes in 2020, the yearly global demand for acetic acid than doubled [2, 12]. In 2021, the market for acetic acid was estimated to be worth $20.6 billion worldwide. Between 2022 and 2030, it is predicted to multiply at a compound annual growth rate of 4.9% [4]. A significant amount of the acetic acid is recovered via recycling of aqueous solutions from industry [13].

A considerable amount of water containing acid can be produced by chemical reactions utilizing acetic anhydride as a reactant or an extractant. Fermentation techniques and synthetic methods are the primary means for producing acetic acid. These methods produce acetic acid at varied amounts in diluted forms [14-16]. Additionally, acetic acid is present in most effluent streams, but in trace amounts. To get the typical glacial acetic acid, this calls for additional processing procedures [17, 18]. Another valuable addition to the industry is the recovery of ethanoic acid from industrial waste [19]. Industry-related wastewater generation has grown to be a significant source of pollution. Waste and both organic and inorganic pollutants are the source of the water contamination. A significant contaminant is acetic acid. Diluted acetic acid is found in waste streams from several chemical and petrochemical businesses. Wastewater from the petrochemical, process, and fine chemical industries contains acetic acid. Wastewater treatment has made extensive use of conventional treatment techniques to eliminate both organic and inorganic components [20-25]. Acetic acid is an essential substance that gets generated via acetaldehyde and Naphtha oxidation along with methanol carbonylation. All these processes include a phase for separating acetic acid from water [26]. Moreover, it is well-known as an integral raw ingredient in the chemical industry. However, in the formation of acetic acid, it frequently coexists with a large amount of water. Demand of highly pure acetic acid in industry, leads the development of highly efficient separation technique of water and acetic acids [27-30]. However, the intricate molecular interaction of the ethanoic acid and water binary system complicates the purifying procedure [31]. Although regular distillation is straightforward and quick to run, it consumes an enormous amount of energy and requires a multitude of column trays. The number of column trays required for azeotropic distillation is less than that required for regular distillation. However, because the separating agents are not vaporized during the extractive distillation process, the energy consumption is minimal [32]. Acetic acid has historically been a prominent fatty acid in manufacturing, traditionally obtained through wood distillation and sugar fermentation to produce ethanol [33, 34]. The shift to petroleum-based resources in 1916 marked a pivotal moment, utilizing acetaldehyde from acetylene derivatives for acetic acid production. Presently, global efforts aim to convert agricultural and forestry waste into efficient chemicals to mitigate pollution from petroleum feedstocks. However, the fermentation process yields only 10% of desired compounds due to product inhibition, and both agriculture and industry heavily consume the limited natural water supply, leading to substantial sewage production. Manufacturing processes for acetic anhydride, polyethylene terephthalate, vinyl acetate monomer, pure terephthalic acid, and petrochemicals result in wastewater containing acetic acid. This dual challenge encompasses both the production of a crucial industrial component and the purification of wastewater laden with acetic acid. Furthermore, the production of acetic acid often yields watery byproducts, necessitating water removal for acetic acid purification. The dehydration process, vital for the pharmaceutical industry, encounters challenge due to the intricate interaction between acetic acid and water molecules, featuring both straight and branched hydrogen bonds [35].

It is not an easy task to mitigate environmental pollutant, particularly organic contaminants such as carboxylic acids, of growing environmental concern. Hence, it is necessary to separate this acids from aqueous solutions for economic reasons and because it is environmentally favorable. The first three groups of carboxylic acids, are primary feedstock for core chemical engineering industrial processes [36-39]. These carboxylic acids find application at different stages of fungicide manufacturing, food processing, medicines, and pharmaceutics. Residues of these chemicals are found in the effluent process streams upon extensive use [40-42]. The process of acetic acid dehydration is crucial for the manufacturing of aromatic acids like terephthalic acid or cellulose acetate. To separate acetic acid and water will be impractical via simple distillation because as it will require numerous equilibrium phases. Since the mixture forms tangent pinch towards clean water end, hence the more suitable is heterogeneous azeotropic distillation using entrainer [43].

Ion exchange, solvent extraction, solvent pervaporation, reactive extraction, electrodialysis, membrane-based extraction, and direct distillation are a few techniques for physical and chemical separation. Acetic acid has been recovered and separated from its aqueous phase using a combination of adsorption and precipitation [44-50]. Acetic acid levels in industrial streams can differ significantly. For acetic acid feed concentrations exceeding 50% (w/w), the traditional distillation technique is employed [48]. Distillation-based separation is loaded with disadvantages like high energy consumption and a greater number of trays columns. Ion exchange and adsorption techniques are mostly used for low input concentrations. Concerns in these activities include regeneration, adsorbent choice, and disposal of used matrices [49]. Membrane technology enables adaptability and can be utilized for low concentrations at various scales. It does, however, have significant drawbacks, namely fouling and disposability. Periodic cleaning is required to prevent membrane fouling, which also uses a lot of energy. Considering these factors, solvent extraction has drawn a lot of interest for acetic acid recovery since it meets standard acetic acid concentration requirements in industrial applications [51]. Yan *et al*. [52] studied low-transition temperature mixtures (LTTMs) as novel solvents for separating azeotropic isobutanol/isobutyl acetate. The authors use COSMO-RS modeling and experimental validation to study selectivity, capacity, and mechanism of separation. They find that hydrogen-bonding interactions between LTTMs and isobutanol disrupt the azeotrope, improving relative volatility. Some of the similar work is also conducted by other researchers to addresses separation of a complex ternary industrial mixture containing isobutyl acetate, acetic acid, and isoamyl acetate. It combines experimental vapor–liquid equilibrium (VLE) data with process simulations to evaluate distillation schemes. The paper highlights difficulties due to close boiling points and azeotropy, and proposes optimal column configurations. For your dataset, this illustrates that industrial feed impurities significantly affect TAC and energy duty; it suggests that multicomponent optimization (not just binary azeotropes) is essential [53]. Zhang *et al.*, studies MTBE/methanol azeotrope separation via extractive distillation using different solvents. Both molecular simulations and Aspen Plus modeling were employed to evaluate entrainer effectiveness and column energy demand. This is highly relevant to your MTBE extractive distillation entry, which already shows low TAC and duty compared to azeotropic cases [54]. Similarly extractive distillation was used solvent for isobutyl acetate / isobutanol separation, using Aspen simulations, they design conventional extractive columns [55].

In the present study, the focus is to optimize the process of acetic acid recovery from the industrial waste. Also, the investigation explores the purity of separated acetic acid along with the comparative analysis of simple and azeotropic distillation, where entrainer will be added as third component. Finally, the process optimization incudes the yield, purity and cost involved. The whole study is conducted using Aspen Plus v14 software.

2. Methods and Process Formulations

2.1. Evaluation & Selection of Specifications

Process simulation is a model-based software representation of technical processes such as physical, chemical, biological, and other unit operations. It can be applied for planning, creating, analyzing, and improving processes. There are many simulations software available in the market, such as Aspen HYSYS, Aspen Plus, CHEMCAD, and DWSIM, etc. In this study, Aspen Plus V14 has been used to simulate the processes. The main steps in the simulation process involve identifying chemical components, selecting a thermo-dynamic model, figuring out plant capacity, choosing suitable operational units, and specifying input conditions (flowrate, temperature, pressure, and other conditions).

2.1.1. Selection of Components

The ASPEN PLUS component database has all the essential components needed for modelling of the process, including water, acetic acid, vinyl acetate, isobutyl acetate. Water and acetic acid were the main components for ordinary distillation. However, vinyl acetate and isobutyl acetate were chosen as the entrainers for the azeotropic distillation of water and acetic acid.

2.1.2. Selection of Property Packages

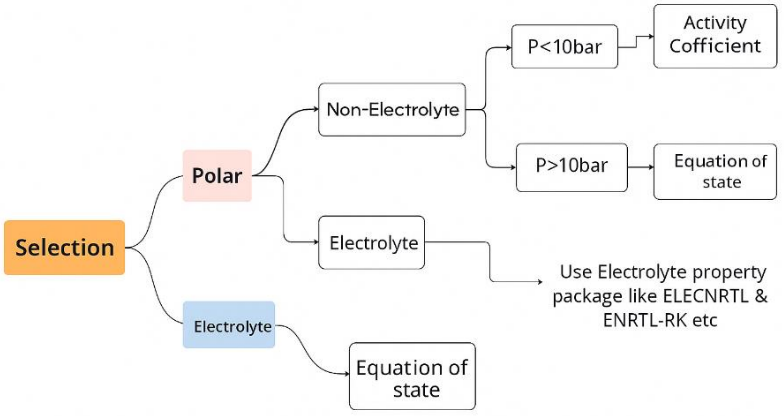

Figure 1: General selection criteria for property package.

Based on the Fig. (**1**), we know that the selection of property package involves primarily the checking of components whether they are polar or non-polar. Next, we need to identify which model we will use either Equation of state or Activity coefficient model according to our components. In case of non-polar solvents, we simply apply equation of the state model. In contrast, when we deal with polar components, we need to further classify whether the component is electrolyte or non-electrolyte. For the case of electrolyte, we use property package like ELECNTRL or ENRTL-RK. In the case of non - electrolyte, pressure of the process taking place is also checked. If it is less than 10 bar then we employ activity coefficient model and conversely for processes at more than 10 bar pressure we prefer equation of state model. Based on this criterion, we found two property packages namely- nonrandom two-liquid (NRTL) activity coefficient model and NRTL accompanied with Hayden-O'Connell (NRTL-HOC). We will validate both and then we will select according to our requirements.

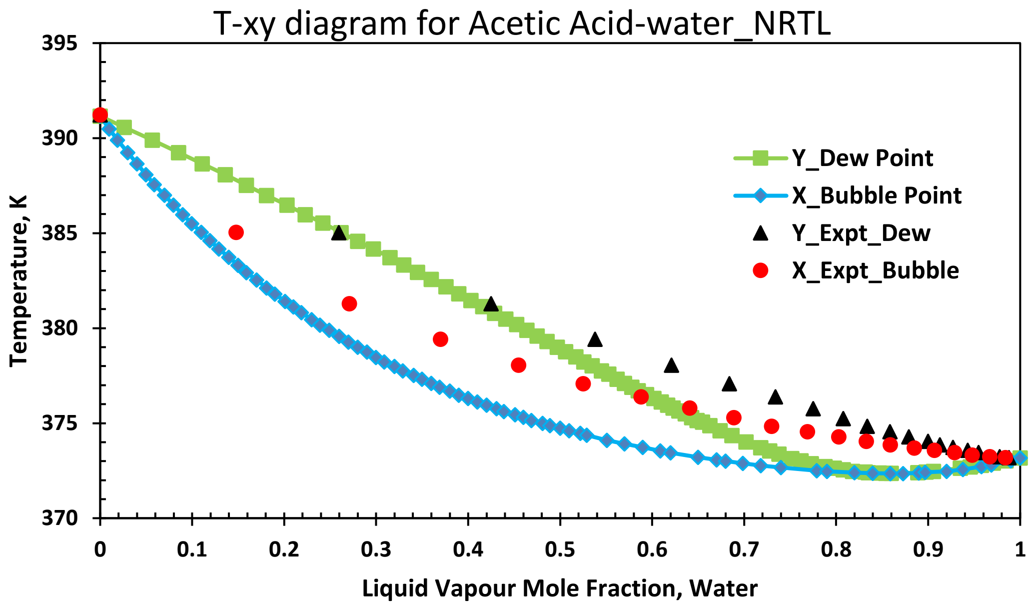

Figure 2: T–x–y diagram of the acetic acid–water system with experimental and calculated bubble and dew points.

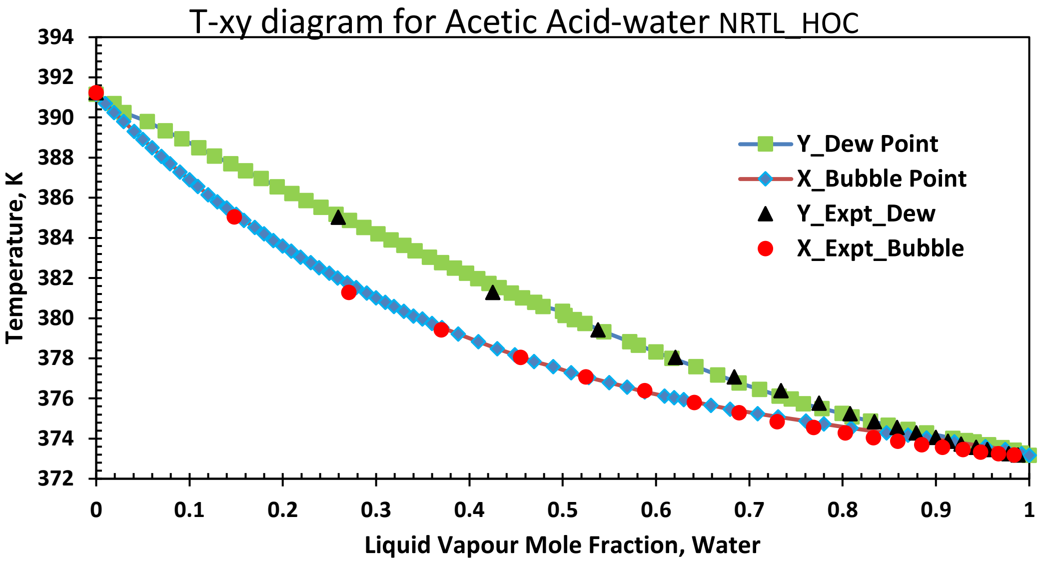

Figure 3: T–x–y diagram of the acetic acid–water system with experimental and calculated bubble and dew points.

The experimental data for various binary VLE is already reported in ASPEN PLUS and its results were compared with the obtained results of NRTL in Fig. (**2**), as well as NRTL-HOC in Fig. (**3**). It was found that the results of NRTL-HOC thermodynamic /activity model were quite matching the reported experimental VLE data. So, NRTL-HOC method was selected for carrying out the simulation. We have also seen NRTL-HOC in [56], Aspen Plus comes with a set of built-in NRTL parameters for the ternary systems of acetic acid-water-vinyl acetate and acetic acid-water-ethyl acetate. The NRTL values for the acetic acid-water-methyl tert-butyl ether system are from [57], while the NRTL parameters for the acetic acid-water-isobutyl acetate system are taken from [58]. The NRTL parameters are tabulated in Table **1-4**.

Table 1: NRTL model parameters for the ternary mixture of acetic acid, water, and vinyl acetate.

Component i	Component j	a_ij	a_ji	b_ij	b_ji
HAC	Water	-1.9763	3.3293	609.8886	-723.888
Water	VAC	0	0	1364.6	415.7
HAC	VAC	0	0	38.385	189.2358

Table 2: NRTL interaction parameters for the acetic acid–water–vinyl acetate ternary system.

Component i	Component j	a_ij	a_ji	b_ij	b_ji	α_ij
Water	HAC	0	0	-211.31	652.995	0.3
VAC	Water	0	0	1809.079	489.609	0.2505
VAC	HAC	0	0	90.268	194.416	0.3

Table 3: NRTL model interaction parameters for the ternary mixture of acetic acid, water, and ethyl acetate.

Component i	Component j	a_ij	a_ji	b_ij	b_ji	α_ij
Water	HAC	-1.9763	3.3293	609.8886	-723.8881	0.3
VAC	Water	9.4632	-3.7198	-1705.68	1286.138	0.2
VAC	HAC	0	0	-235.279	515.8212	0.3

Table 4: **NRTL interaction parameters (aij, aji, bij, bji, αij) for the ternary system consisting of acetic acid, water, and methyl tert-butyl ether.**

Component i	Component j	a_ij	a_ji	b_ij	b_ji	α_ij
Water	HAC	0	0	-307.16	597.97	0.3
EA	Water	0	0	1307.33	707.56	0.3
EA	HAC	0	0	-47.36	-113.15	0.3

2.2. Design Constraint

Here, the problem arises when we observe tangent pinch in the water – acetic acid binary system VLE at the pure water end. Due to tangent pinch condition, it is not practically possible to separate water and acetic acid binary mixture by ordinary distillation as the required number of trays will be infinite. So, we need to shift our focus from ordinary distillation to other alternatives such as azeotropic and extractive distillation. In azeotropic distillation, the selection of good entrainer is a major task as the ease of separation as well as the product purity is directly affected by the entrainer. Similarly, we need to select such a solvent in extractive distillation which can yield effective results and easily solve our purpose. The XY- Diagram showing the tangent pinch condition for the acetic acid-water binary mixture is as shown in Fig (**4**).

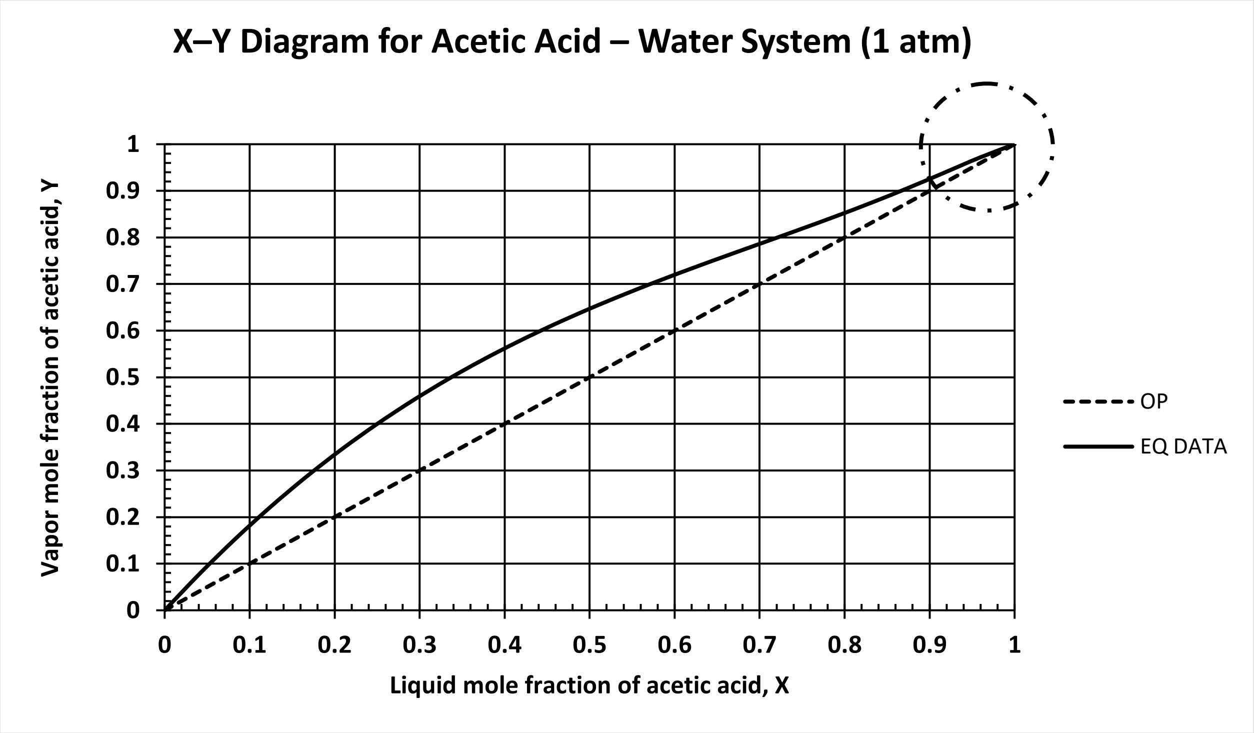

Figure 4: XY-diagram of acetic acid-water binary mixture.

2.3. Analysis and Feature Finalization Subject to Constraints

Modern simulation platforms, when utilized effectively, can generate reliable data on process behavior owing to their comprehensive thermodynamic models, advanced computational algorithms, and extensive component libraries. In the present study, ASPEN PLUS was employed to perform the process simulations. The software offers a wide selection of thermodynamic property packages to enhance accuracy; hence, the proper identification and application of the most suitable property package is crucial for reliable simulation outcomes.

3. Results and Discussion

3.1. Ordinary Distillation

In the context of ordinary distillation, the VLE (Vapor-Liquid Equilibrium) diagram for the acetic acid-water binary mixture, modeled by NRTL-HOC shown in the Fig. (**4**), reveals a distinctive tangent pinch near the pure water end, highlighted within a black dotted circle on the XY diagram in the Fig. (**4**). T-x-y diagram of acid and water is depicted in Fig. (**5**). Fig. (**6**), is the schematic representation of ordinary distillation unit.

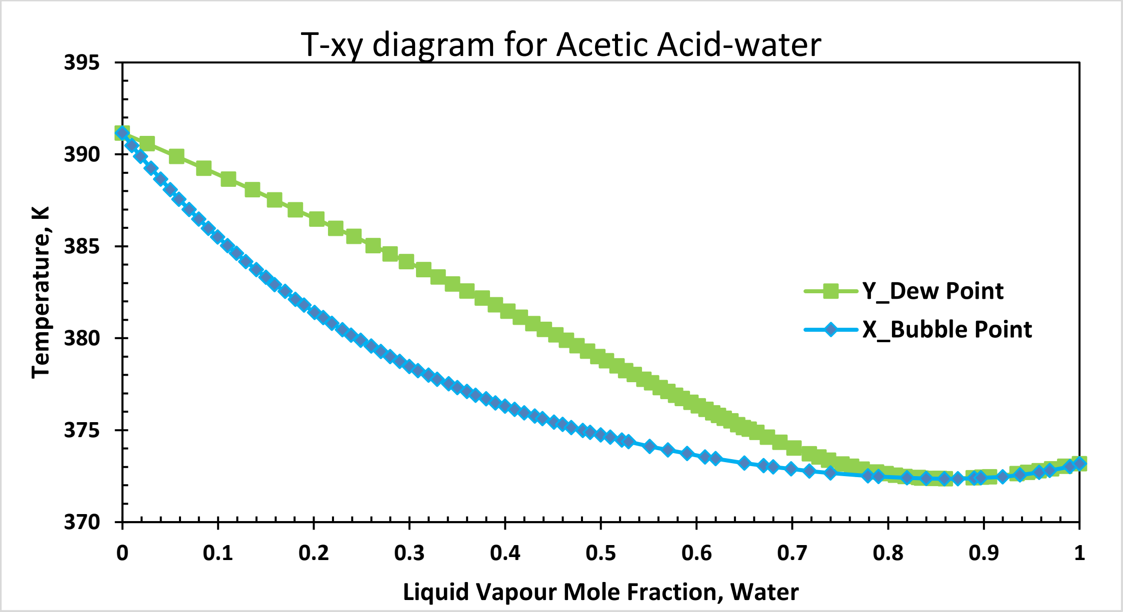

Figure 5: Temperature–composition (T–x–y) diagram of the Acetic Acid–Water binary system, illustrating bubble point and dew point variations with the mole fraction of water.

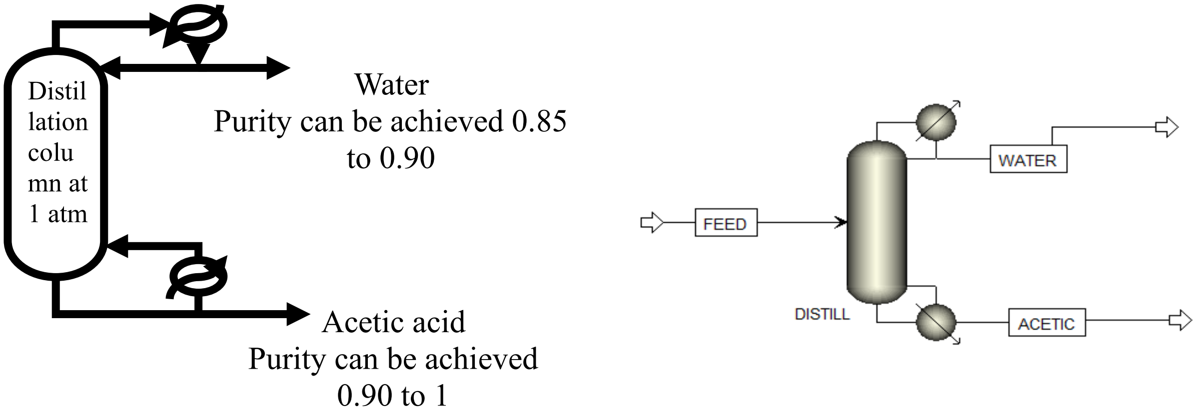

Figure 6: Distillation column schematic for separating acetic acid and water.

Due to this tangent pinch point, the purity of water which can be achieved is around 85 to 90%. To increase the purity and for getting more efficient results, we need to use infinite trays for separation which is practically not possible at the industrial scale. So, we prefer to go with the other alternatives. We obtain water and acetic acid in our simulation as top and bottom product respectively. The purity of water obtained is 86% in the top section and 92% of pure acetic acid was obtained in the bottom. To develop more purified acetic acid, we need to shift to other methods rather than simple distillation.

3.2. Azeotropic Distillation

The two entrainers in this work, isobutyl acetate and vinyl acetate, is used. A minimum-boiling water azeotrope is released from the column top, and highly pure acetic acid is recovered at the bottom. At the top of the column the tangent pinch of pure water can be prevented with this column design. The heterogeneous entrainer-water azeotrope can be sent to a decanter for the formation of two liquid phases. To supply sufficient entrainer within the column, the organic phase is recycled back to the azeotropic column. The further reduction in entrainer residue in water, the aqueous phase, which is primarily composed of water, if supplied to stripping column. The distillate from the stripping column can also be recycled back into the decanter at the entrainer-water azeotrope.

The ternary of all three components is displayed in Fig. (**7**-**9**), respectively. The feed condition and the composition of acetic acid, water and entrainer is shown Table **6**. Under ideal circumstances, the distillation column's top vapor composition should be at the entrainer-water azeotrope, while Fig. (**7**) and (**8**) show that the column bottom composition should be extremely near to the pure acetic acid corner. The mass balance of the distillation column and the feed composition allow for the determination of the organic reflux flowrate, which may be estimated by intercepting the mass balance lines of the two inlets and exits.

The reflux stream's flowrate is high since the organic reflux is closer to the interception site. The system in Chien *et al*. (2004) uses a single column. The proposed feed composition and stipulated product purities differ from this work; hence additional purification of the water by-product requires the use of a second water stripping column. In every instance, the entrainer makeup can be overlooked with the help of a stripping column. All the results of this process are shown in the Tables **5** and **6**.

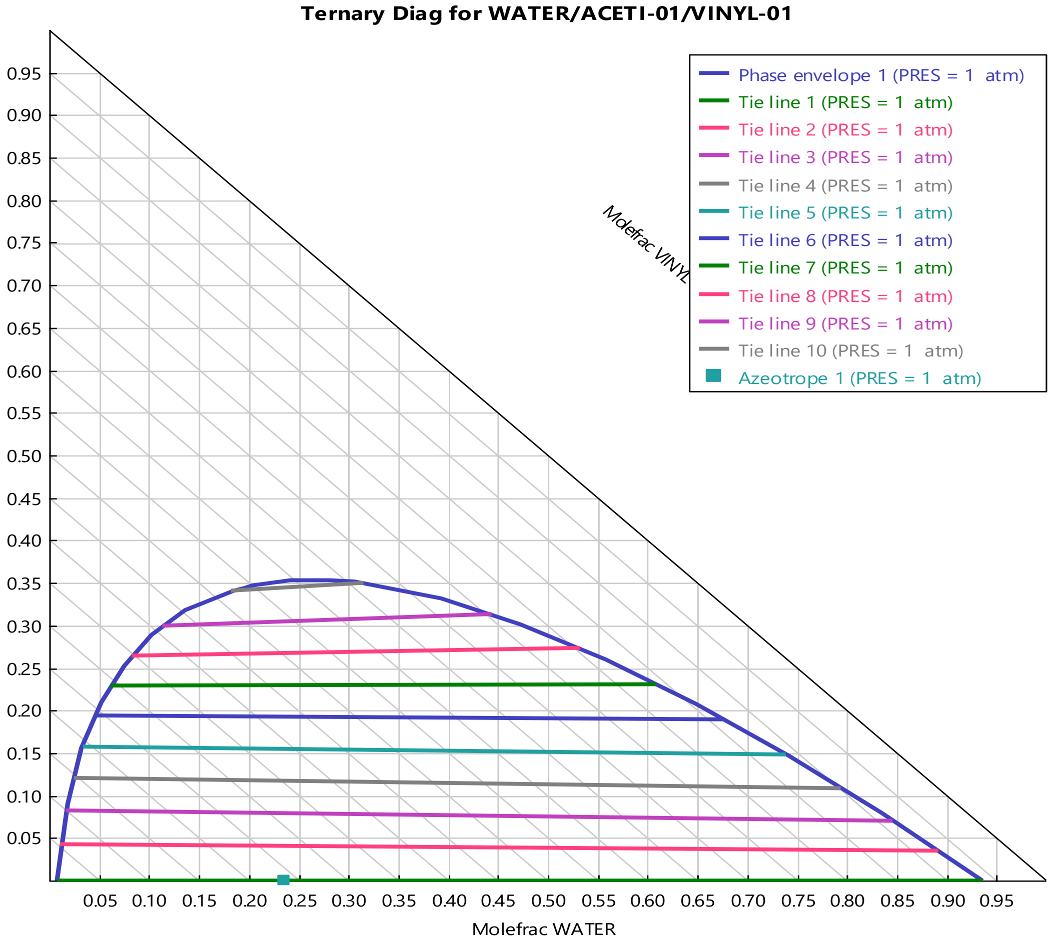

Figure 7: Ternary composition diagram (mass basis) for the Acetic Acid–Water–Vinyl Acetate system.

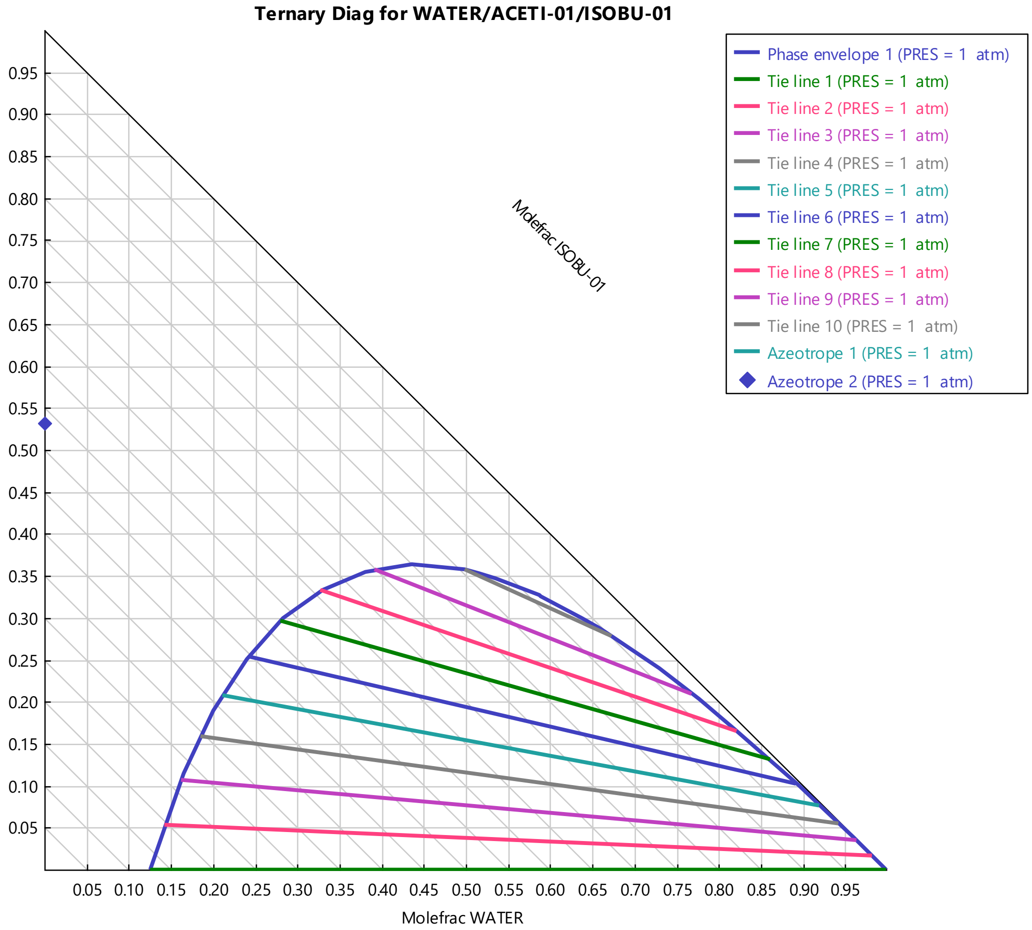

Figure 8: Mass-based ternary diagram of Acetic Acid–Water–Isobutyl Acetate.

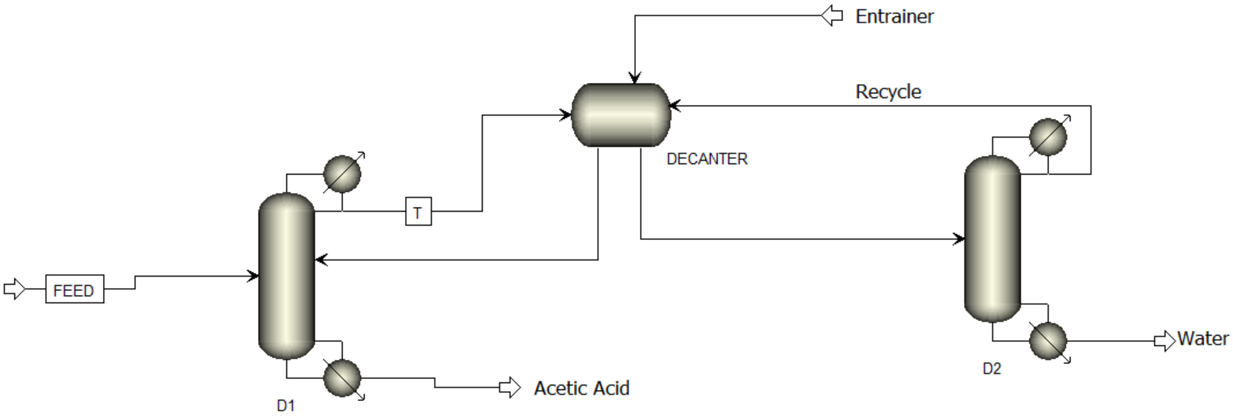

Figure 9: Azeotropic distillation flowsheet.

Compared to the VAC case, the IBA system uses a lot less energy overall. Consequently, it is preferable to use isobutyl acetate as an entrainer in the industry rather than vinyl acetate. When comparing systems using the acetate of vinyl and isobutyl, it is preferable to select the entrainer that creates an azeotrope with a composition that has a higher percentage of water. Because of its increased ability to transport water to the column top and isobutyl acetate a superior entrainer is compared to vinyl acetate.

3.3. Extractive Distillation

A hybrid extraction/distillation process involves first performing a liquid-liquid extraction and then moving on to an azeotropic distillation step in Fig. (**10**). High-purity acetic acid (HAC) is recovered as the bottom product of Distillation Column D1, which treats the extract stream leaving the extractive distillation column (EX). This stream is rich in both HAC and solvent. In parallel, the raffinate stream, composed mainly of water with only minor HAC content, is sent to Distillation Column D2 (stripping column), where clean water is obtained as the top product.

The distillate streams from D1 (solvent–water mixture) and D2 (water-rich phase) display liquid–liquid immiscibility and are separated in the decanter (DEC). In this step, the organic phase—predominantly solvent—is recycled back into the extraction column after passing through Mixer M1 and heat exchanger C1, which reduces the demand for fresh entrainer. The aqueous phase from the decanter is merged with the raffinate and then processed in D2, as their compositions are nearly identical.

Among the critical design factors—besides the number of stages and feed tray locations in each column—the solvent-to-feed ratio in EX plays the most significant role. A smaller ratio results in greater HAC losses in the raffinate, while a larger ratio increases the energy duty of D1 because of the higher solvent circulation. Consequently, this ratio should be treated as an outer-loop optimization variable. Furthermore, the number of theoretical stages in EX directly influences the separation efficiency and must be carefully optimized.

For entrainer selection, low-boiling solvents such as methyl tert-butyl ether (MTBE) and ethyl acetate (EA) are commonly considered. Their choice depends on azeotrope characteristics, cost, solubility in water, and distribution behaviour. While both solvents exhibit similar distribution coefficients for HAC, the energy required for solvent recovery in D1 strongly impacts process economics. Owing to its lower vaporization enthalpy and the smaller water fraction in its azeotrope, MTBE generally leads to lower energy consumption compared to EA, making it a more efficient solvent for the Aspen-based process flowsheet.

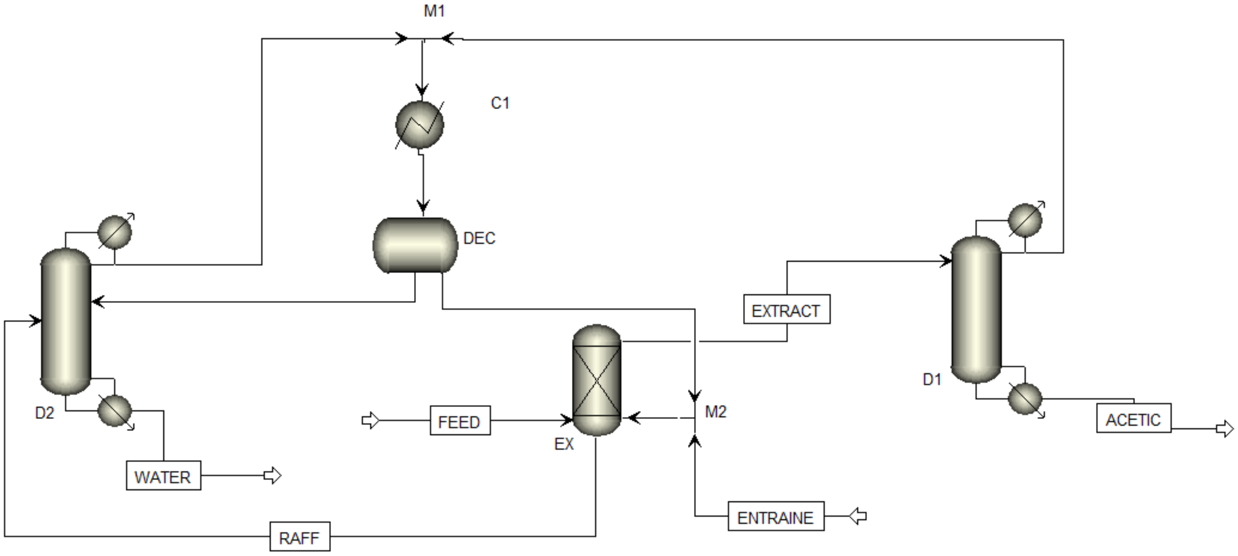

Figure 10: Aspen Plus process flowsheet for acetic acid–water separation via extractive distillation.

Liquid–liquid extraction, also known as solvent extraction, is a separation method that exploits the differing solubilities of compounds in two immiscible liquid phases, typically an organic solvent and water. In an azeotropic distillation sequence, the introduction of a suitable solvent with water results in the formation of a minimum-boiling azeotrope, as illustrated in Fig. (**11**) and (**12**). Using an extraction column, residual concentrations as low as 0.1-0.5 wt% can be achieved. A detailed overview of the optimized Aspen Plus® simulations for both the EA and MTBE solvent systems is presented in Fig. (**10**) and Table **5**-**7**, with the principal stream compositions mapped on the ternary diagrams shown in Fig. (**11**) and (**12**).

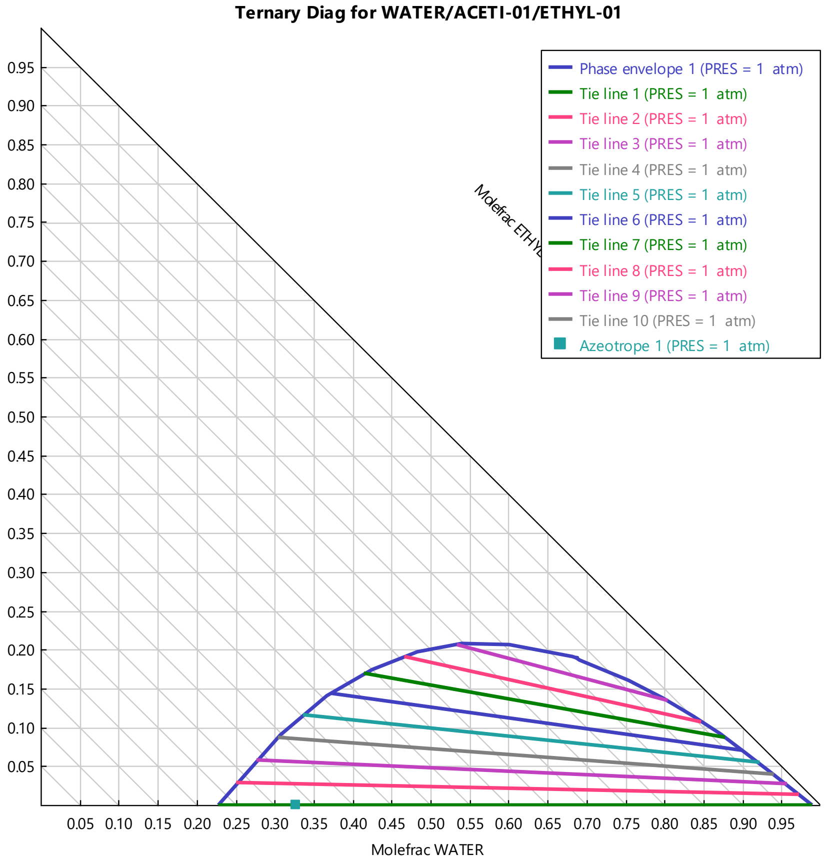

Figure 11: Ternary phase diagram on a mass basis for the acetic acid–water– Ethyl Acetate (EA) system.

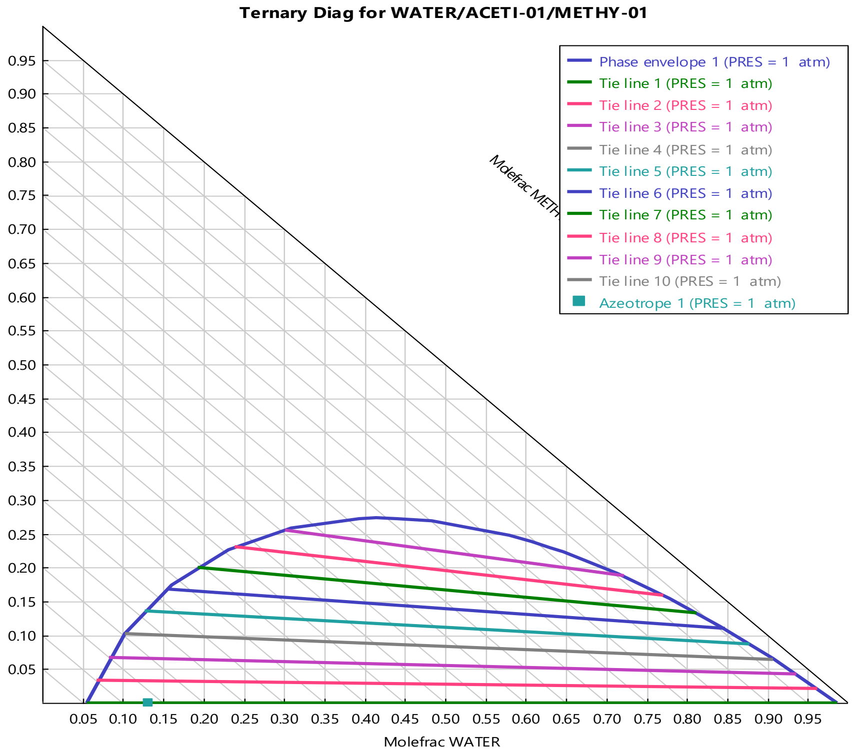

Figure 12: Ternary phase diagram on a mass basis for the acetic acid–water–methyl tert-butyl ether (MTBE) system.

Table 5: Column trays, duty, and total annual cost (TAC).

	Column Tray			**Total Cooling Duty (MW)**	**Total Heating Duty (MW)**	**TAC($\$10^6$/yr)**
	Distillation Tray		Extraction tray			
	Column 1	Column 2				
Simple Distillation	38					
Azeotropic Distillation						
Vinyl Acetate	35	18		-209.35	209.09	28.29
Iso-Butyl Acetate	20	18		-107.95	107.59	13.64
Extractive Distillation						
Ethyl Acetate	42	13	35	-82.65	79.26	11.84
Methyl tert-butyl ether (MTBE)	23	9	20	-43.65	39.54	8.73

Table 6: Details of various parameters used in simulation studies.

	Temperature (T)	**Pressure (ATM)**	**Flowrate (kg/hr)**	**Mass Fraction (Acetic Acid)**	**Mass Fraction (Water)**	**Mass Fraction (Entrainer/ Solvent)**
Simple Distillation Process						
Feed	49	1	12000	0.4	0.6	
Water	100.433	1	7956.2	0.864	0.135	
Acetic Acid	109.512	1	4043.8	0.921	0.078	
Azeotropic Distillation Vinyl Acetate						
Feed	49	1	12000	0.4	0.6	
Acetic Acid	117.264	1	4568.25	0.984	Trace	Trace
Water	99.889	1	7631.72	Trace		Trace
Entrainer	40	1	106.26			1
Iso-butyl Acetate						
Feed	49	1	12000	0.4	0.6	
Acetic Acid	117.264	1	4236.25	0.986	Trace	Trace
Water	99.889	1	7431.72	Trace	0.99	Trace
Entrainer	40	1	89.26			1
Extractive Distillation Ethyle Acetate						
Feed	49	1	12000	0.4	0.6	
Acetic Acid	117.264	1	4236.25	0.986	Trace	Trace
Water	99.889	1	7431.72	Trace	0.99	Trace
Entrainer	40	1	164.39			1
MTBE						
Feed	49	1	12000	0.4	0.6	
Acetic Acid	117.264	1	4712.39	0.99	Trace	
Water	99.889	1	7359.85	Trace	0.99	
Entrainer	40	1	73.65			1

Table 7: Parametric details of azeotropic distillation.

Azeotropic Distillation					
Equipment	**No. of Trays**	**Reflux Ratio**	**Column Pressure (ATM)**	**Flow Rate**	**Convergence Criteria**
Extract	31	NA	1	12000 kg/hr	0.0001
RadFrac_D2	30	1.6	1	260.3 kg/hr	0.0001
RadFrac_D1	35	1.89	1	11749.7 kg/hr	0.0001

4. Conclusions

The separation of acetic acid from aqueous mixtures presents significant challenges due to the tangent pinch phenomenon encountered in conventional distillation, leading to high energy consumption and limited product purity. While ordinary distillation achieved only 92.1% acetic acid and 86.4% water, the use of azeotropic distillation with entrainers markedly improved separation performance. Vinyl acetate produced 98.4% acetic acid and 99% water, whereas isobutyl acetate slightly outperformed it, yielding 98.6% acetic acid and 99% water. Extractive distillation offered even greater advantages, with ethyl acetate providing 98.2% acetic acid and 99% water. Among the solvents tested, methyl tert-butyl ether (MTBE) proved to be the most effective, achieving 99% purity for both acetic acid and water, with the lowest energy demand, reduced tray requirements, and favorable solvent properties. Overall, MTBE-based extractive distillation demonstrates the most efficient and sustainable approach, combining superior separation performance with reduced operational costs and energy consumption, thereby offering a promising pathway for industrial-scale acetic acid purification.

Conflict of Interest

The authors declare no competing financial interest.

Funding

The study received no financial support.

Acknowledgments

The authors acknowledge the support received from the Department of Chemical Engineering, Chandigarh University, Mohali, Punjab, India. Most of the computational work has been carried out in the computational laboratory at the Department of Chemical Engineering of the Chandigarh University, Mohali, Punjab, India.

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