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Simulation of Extractive Distillation using ChemSep

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Abstract
Isopropyl alcohol, or IPA, is a highly versatile solvent widely applied in cosmetics, dental care, pharmaceuticals, and electronics such as computers and digital cameras. However, manufacturing processes often allow water to contaminate IPA, which, in turn, influences the quality of IPA. This research paper not only elaborates on the recovery and purification of the IPA that has been contaminated and focuses on economic and environmental reasons but also aims to make a significant contribution to the ongoing research efforts in the field. Furthermore, it gives a summary of presently available separation techniques and illustrates a comparative study between them. These techniques are distillation, azeotropic distillation, extractive distillation, membrane separation, and adsorption. By weighing the merits and demerits of each method, the study sets out to make a constructive contribution to the ongoing research efforts of more efficient and sustainable methods in the purification of IPA.

INTRODUCTION

Isopropyl alcohol, also called isopropanol or 2-propanol, is a colourless and clear liquid with a slight odour and water-soluble, ethanol-soluble, and chloroform-miscible materials. It is a gem in many fields, from pharmaceuticals and cosmetics to electronics. The use of IPA as a solvent has made its mark in drug, medicine, and personal care item manufacturing. This, plus its ability to dissolve a broad range of polar and non-polar contaminants, is thus not distilled IPA with silver vesicles from silver salt as an intermediary.[1–6]

The total international sales of IPA are in step with the upward expansion of the pharmaceutical, mineral water, and electronics sectors highlighted below. The world market of isopropyl alcohol increased by 4.5% between 2022 and 2030, thus achieving 54 billion dollars worth, as stated in the report by Grand View Research. This fact once again underlines the importance of keeping the supply of IPA reliable and cost-effective.

Water contamination in IPAs may occur during the extraction or refining process of various industrial chemicals. Leaks, oxidation, improper handling, and other causes can cause water in the final product. Locating and addressing the contamination paths is of the highest priority for IPA developers to maintain the purity and quality of IPA in their original applications.

ECONOMIC AND ECOLOGICAL JUSTIFICATIONS

The combinations of IPA are made by a selection of materials that change the final production price, and they are raw materials, energy, and strict regulations. In the environmental aspect, manufacturers can achieve huge savings through the reduction of contaminated IPA costs by cleaning and getting high-quality IPA back on the market. Recycling and reuse of IPA (Isopropyl alcohol) can help to reduce waste, avoid disposal costs, and save resources, thus helping the companies to be more profitable and competitive. By reusing IPA, companies are able to cut down their environmental impact and adhere to stricter environmental laws. The use of pure IPA in different applications might bring about enhanced product quality and performance, thus, customers and the environment also benefit.

Methods Of Ipa Separation From Ipa- Water Mixture

Selective Techniques for the separation of IPA are the most energy-efficient and sustainable techniques; several options are represented in the published works for the dissociation of IPA from water:

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1. Distillation: A robust approach is a net distillation, a process that exploits the differences between the boiling points of its constituents in a mixture. The distillation process, which is the separation of IPA from water, might require significantly keen awareness, and, in the worst cases, energy might not be enough to do this.
2. Azeotropic Distillation: A specific method is to add a third component, azeotrope, in the primary IPA-water mix to create an entirely new entity by going along with one of the former, which can then be split. The process of distillation is feasible in this instance, allowing the participants to take the action of selection, and instead, they have to recover the entrainer properly.
3. Extractive Distillation: By adding a solvent with a high boiling point to the IPA-water mixture, one can change the volatilities, and the separation can then be done. The procedure is usually more cost-effective than pressure swing distillation in the case of high boiling point mixtures. Usually, a better solvent recovery is achievable compared to azeotropic distillation.
4. Membrane Separation: The use of semi-permeable membranes, the pathway that is responsible for the sulfide to pass through on a basis different from the sulfate, may be regarded as one process that merits further consideration in the environmental technology sector.
5. Adsorption: The selective adsorption process allows IPA to be adsorbed onto a solid adsorbent. Then, desorption occurs, followed by the recovery of IPA. Adsorption could even possibly replace distillation techniques. This could not only reduce energy consumption but also simplify starting a process.

The advantages and limitations of every method of separation, each one having its virtues and payoffs. The selection of the best method is a matter of the scale of a given operation, energy efficiency, cost savings, and environmental issues. When choosing a method to separate substances, it's like picking the right tool for a job. Factors like how big the job is, how much energy it needs, how much it costs, and how it affects the environment all play a role. **Table 1** compares different methods based on how well they recover the substance, how much they cost, how much energy they use, and how pure the final product is. Distillation and its variations, while offering superior recovery rates and purity levels, often demand significant energy inputs and incur higher costs. In contrast, membrane separation and adsorption, though less energy-intensive and economical, may compromise recovery rates and product purity. The optimal selection for a specific application hinges on a careful evaluation of these trade-offs and the prioritisation of individual requirements.

Table 1: Comparative study of different methods

Method	Recovery Rate	cost	Energy Consumption	Purity level
Distillation	High	Moderate	High	High
Azeotropic Distillation	High	High	High	High
Extractive Distillation	High	Moderate	Moderate	High
Membrane separation	Moderate	Low	Low	Moderate
Adsorption	Moderate	Low	Low	Moderate

In this paper we have explored extractive distillation as a technique to separate IPA-water mixture.

Extractive Distillation[1-5,7–12]

Isopropyl alcohol (IPA) is an inexpensive solvent that is employed in a wide range of industries such from pharmaceuticals and cosmetics to electronics. Still, IPA, during the production process, could be contaminated with water, which, together forms the close-boiling azeotrope, will impede distillation by means of standard distillation techniques. One possible solution is to introduce another component to the process, utilising a method called extractive distillation, which not only proves feasible but also economically beneficial for the entire production

The strategy of extractive distillation involves the use of a third component, known as an 'entrainer' or an incorporating/ extracting solvent, to separate the volatile compositions (IPA and water). By employing this technique, the production from these raw materials becomes more practical as the entrainer forms a new azeotrope with either IPA or water, making them completely pure.

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In an extractive distillation process, there are three significant steps: feed preparation, distillation, and separation. The contaminated IPA-water mixture is introduced into the distillation column along with the chosen entrainer or solvent. The mixture is then heated, and the components are separated based on their boiling points. This results in a change in the relative volatilities of IPA and water. The top product is pure IPA, and the bottom product consists of the entrainer or solvent and the water mixture.

Many advantages are provided by extractive distillation compared to other separation methods, which makes it a perfect choice for IPA-water purification. In the first place, it guarantees a higher yield and reduced waste since it allows the use of an enthalpy entrainer in addition to IPA. Also, the liquor, which serves as an entrainer in the separation of IPA from water with higher purity levels, is added to the final product. In addition, extractive distillation without the maintenance of high pressures and temperatures can be more energy-saving than other methods, such as pressure swing distillation, which may lead to a reduction in operational costs.

During the extractive distillation in the separation of IPA-water, several extractants have been investigated. Ethylene glycol and Dimethyl sulfoxide (DMSO) among them are the most popular. As for ethylene glycol, it is a commonly used entrainer that can form the same-phase azeotrope with water. It is possible to separate and recover high-purity IPA by this method. DMSO (Dimethyl sulfoxide), which is a polar solvent, alters the relative volatilities of IPA and water, facilitating the separation with high purity levels.

Countless studies have been carried out, both with simulation and experiment, aiming to apply extractive distillation technology in the separation of IPA-water. Simulation studies performed with software like Aspen Plus have helped to understand process parameters, energy demands, and product purity percentages obtainable with different trainers. The experimental studies have added to the evidence that extractive distillation can be employed in the recovery of high purity and removal of harmful compounds. Thus, they have confirmed theoretical principles and simulations.

METHODOLOGY

This research employs extractive distillation to separate isopropyl alcohol (IPA) and water mixture using ethylene glycol as the entrainer. Simulations were conducted in DWSIM to model the distillation process. The IPA-water mixture, with equal mole fractions, was subjected to a distillation column under varying conditions. Key variables, such as reflux ratio and feed temperature, were analysed for their effect on the purity of IPA in the distillate. The findings are based on simulations that adjust these operational parameters to achieve optimal purity and energy efficiency. Simulations are carried out in DWSIM.

The binary mixture of IPA-Water has a mole fraction composition of IPA-0.5 (mole/mole) and Water-0.5(mole/mole). Pure ethylene glycol is added as an entrainer. This research employs extractive distillation to separate isopropyl alcohol (IPA) and water mixture using ethylene glycol as the entrainer. Simulations were conducted in DWSIM to model the distillation process. The IPA-water mixture, with equal mole fractions, was subjected to a distillation column under varying conditions. Key variables, such as reflux ratio and feed temperature, were analysed for their effect on the purity of IPA in the distillate. The findings are based on simulations that adjust these operational parameters to achieve optimal purity and energy efficiency.

Table 2: Feed Data

OPERATING VARIABLE	EXTRACTIVE COLUMN
Feed flow Rate (kmol/hr)	100
Entrainer flow Rate (kmol/hr)	100
Feed Temperature (°C)	25
Feed Pressure (atm)	1.3
Entrainer Temperature	72
Entrainer Pressure (atm)	1.1
Distillate Rate (kmol/hr)	50
Molar Reflux Ratio	1
No of theoretical Stages	42

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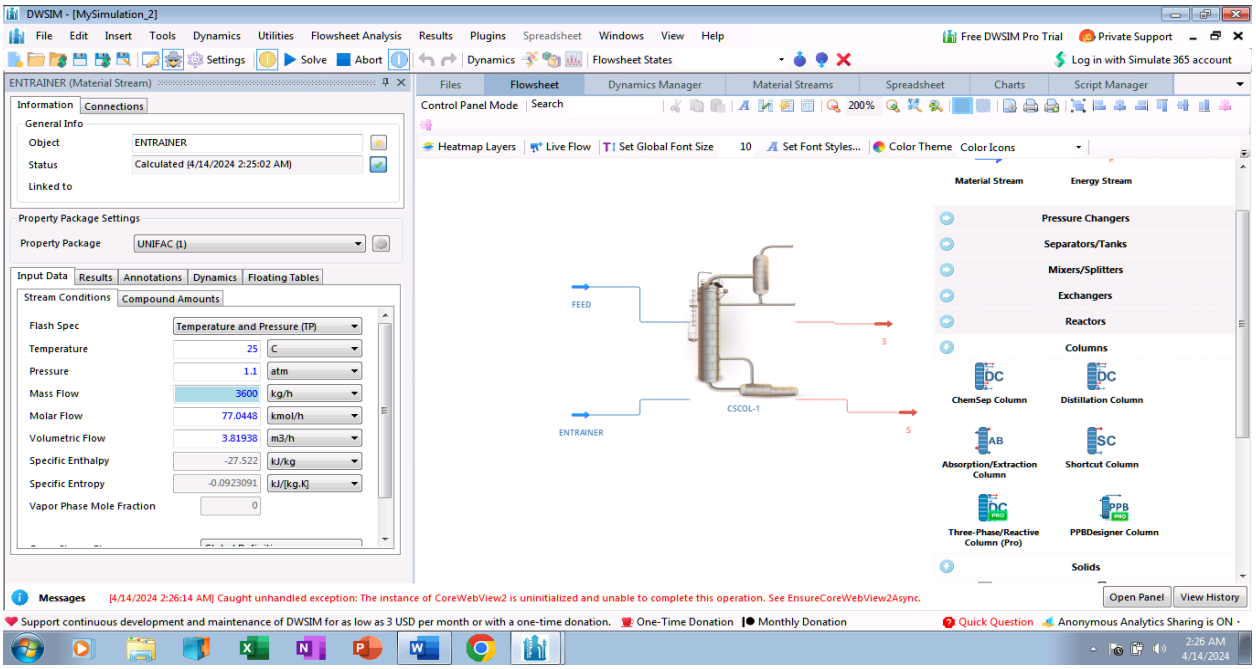

Fig 1: Extractive Distillation model in DWSIM

RESULT AND DISCUSSION

a) Reflux Ratio vs Purity

In the following simulation of extractive distillation using DWSIM, the study of variation of the IPA mole fraction in distillate, i.e., the purity with the reflux ratio, was performed. In this, we estimated purity at different values of the reflux ratio. It is seen that as the reflux ratio increases, the purity also increases. Still, with a further increase in the reflux ratio, the purity reached its maximum value, and further, with the increase in reflux, the purity remained constant.

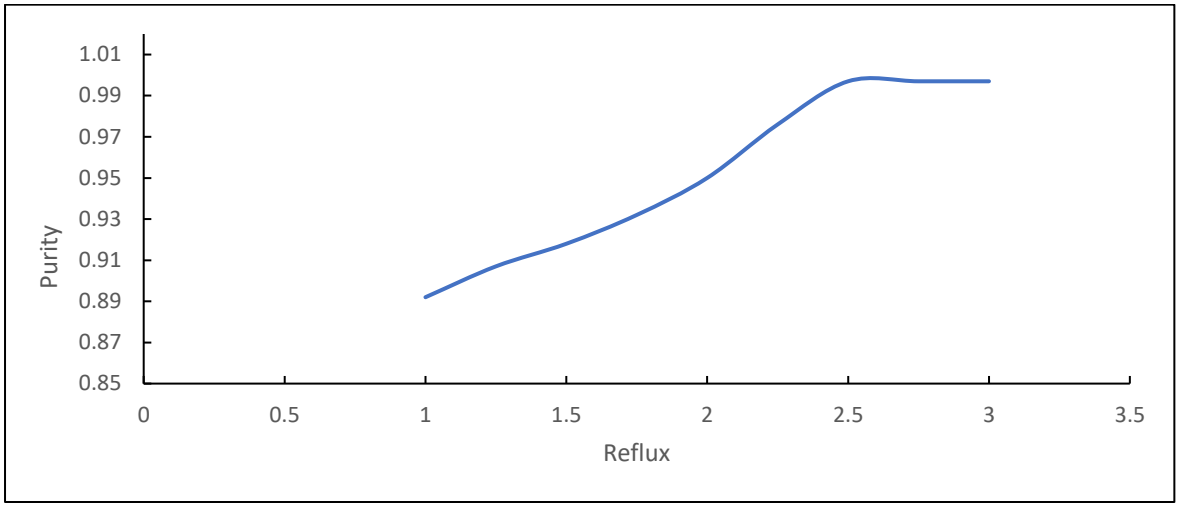

Fig 2. Graph of Purity vs Reflux

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The optimum reflux ratio for the maximum purity obtained was **2.5,** and as the reflux increased, the purity remained the same. The maximum value of the IPA mole fraction is about **99.7%.** It is also evident that no further increase in the purity of the material is observed when the reflux ratio is further increased than 2.5.

b) Feed Temperature vs Purity

Purity is constant at 0.969 at higher R values (1. 5, 2. 0, 2. 5) for all feed temperatures ranging from 15°C to 35°C. At reflux, ratio 1, 0, purity becomes slightly lesser than 0. 871 to 0. 841 with the increase of feed temperature. As per the given data, in extractive distillation, we see that as the feed temperature increases any value of reflux ratio, the purity of the distillate decreases as we increase the temperature. This is because as we increase the temperature, the water, being the less volatile component present in the mixture, also starts to produce vapours, due to which, after a further increase in temperature, more vapours of water will form and move towards the distillate.

Table 4: Data of purity at different feed temperatures

Feed Temp / Reflux	15	20	25	30	35
1	0.871	0.863	0.856	0.848	0.841
1.5	0.945	0.944	0.943	0.942	0.942
2	0.961	0.96	0.959	0.959	0.958
2.5	0.969	0.969	0.969	0.969	0.969

Further, as the reflux ratio value increases for any temperature value, the purity of the mixture increases.

c) Reflux Ratio Impact:

However, in extractive distillation, when increasing the reflux ratio, it is essential to know that the purity of distillate is increased by enhancing the reflux ratio up to a specific limit. There exists a non-linear correlation between the reflux ratio and the product purity with a point of decrease at high values of the former. There is an ideal reflux ratio that one can set to obtain maximum purity and least reflux that will not waste energy.

d) Feed Temperature Influence:

Another observation associated with the purity of the final product is feed temperature, which causes minimal effect as the reflux ratio increases. As the reflux ratio reduces the effect of increasing the feed temperature reduces purity, perhaps because of increased pressure of impurities in the feed. This shows that the process is relatively immune to changes in feed temperature especially when carrying out the process at high values of Reflux ratio.

e) Process Optimization:

This suggests that achieving high purity involves a trade-off with energy consumption, which is influenced by the reflux ratio. Operating within a reflux ratio range of 2.0 to 2.5 can offer a balance, ensuring high-purity production while minimising energy usage.

CONCLUSION:

In conclusion, a reflux ratio of 2.5 achieves the maximum isopropyl alcohol (IPA) purity of 99.7% while providing flexibility in system operation with minimal sensitivity to feed temperature variations. The study identifies a reflux ratio of 2 as the most efficient and cost-effective for eliminating impurities, with further increases offering diminishing returns. Future research could explore the relationship between optimal reflux ratios and energy consumption, as well as investigate the effects of different feed compositions and process stages to enhance system performance.

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