



# A simulation case study on separation of IPA-Methanol-Water mixture by distillation

Dr. Saphal U. Patil<sup>1\*</sup>, Manish C. Lonare<sup>2</sup>, Seema R. Pawar<sup>3</sup>, Pradnya S. Ghode<sup>4</sup>, Prerna D. Khandekar<sup>5</sup>,  
Vedika A. Gosavi<sup>6</sup>

<sup>1,2</sup>Lecturer, Dept. of Chemical Engineering, Government Polytechnic Arvi, Higher & Technical Education  
Department, Govt. of Maharashtra

<sup>3,4,5,6</sup>Lecturer, Dept. of Chemical Engineering, Government Polytechnic Thane, Higher & Technical Education  
Department, Govt. of Maharashtra

\*Corresponding Author: **Dr. Saphal U. Patil**

**Email:** saphalp@yahoo.com

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**Abstract:** The present work focuses on the simulation and analysis of the separation of an Isopropyl Alcohol (IPA)–Methanol–Water mixture using distillation with Dimethyl Sulfoxide (DMSO) as an entrainer. Due to the close boiling points and non-ideal vapor–liquid equilibrium behavior of IPA and methanol, conventional distillation becomes inefficient for achieving high-purity separation. In this study, a three-column extractive distillation process was simulated for efficient methanol separation, IPA recovery, and DMSO solvent recycling. The feed mixture consisted of 40 wt.% IPA, 40 wt.% methanol, and 20 wt.% water, while DMSO was introduced as the extractive solvent. The simulation results demonstrated that methanol purity of 99.25 wt.% and IPA purity of 99.65 wt.% were achieved. Additionally, DMSO recovery of approximately 99.99 wt.% was obtained with negligible solvent losses. The results confirm that extractive distillation using DMSO is an effective and industrially viable technique for the separation of IPA–Methanol–Water systems.

**Keywords:** IPA, Methanol, Water, DMSO, Simulation



## Introduction

Isopropyl alcohol (IPA) is widely used as a solvent, disinfectant, and cleaning agent in chemical, pharmaceutical, and petrochemical industries. Recovery and purification of IPA from industrial waste streams is an important area of research because solvent recovery reduces operational cost and minimizes environmental impact [1-2]. Typical waste streams generated in such industries contain mixtures of IPA, methanol, and water. Separation of these components is challenging due to the formation of azeotropes and the close boiling points of the alcohols. IPA forms a minimum-boiling azeotrope with water at atmospheric pressure containing approximately 68.1–67.5 mol% IPA, with a boiling temperature of about 80.3–80.4°C [1,3]. As a result, conventional distillation alone is not sufficient for obtaining high-purity IPA. In addition, methanol is itself a valuable industrial solvent and its recovery is also economically significant.

In the chemical and petrochemical industries, the separation of azeotropic and close-boiling liquid mixtures remains one of the major challenges in downstream processing[4-6]. The IPA–Methanol–Water ternary system is frequently encountered in solvent recovery operations, pharmaceutical manufacturing, and chemical processing industries. Conventional distillation methods are generally ineffective for this system because of the complex vapor–liquid equilibrium behavior and the small difference in boiling points between IPA and methanol[1,3,5].

Extractive distillation is considered an effective technique for separating such non-ideal mixtures[4-5]. In this method, a high-boiling solvent known as an entrainer is added to alter the relative volatility of the components without forming additional azeotropes. Dimethyl sulfoxide (DMSO) is recognized as an excellent entrainer because of its high boiling point, good thermal stability, low volatility, and strong affinity toward polar compounds such as water and methanol. In the present study, DMSO was employed as the extractive solvent for the separation of IPA and methanol from the IPA–Methanol–Water mixture.

Most of the earlier studies reported in the literature mainly focused on the separation of IPA–Water systems[1-5]. However, limited work has been reported on the simultaneous recovery of IPA and methanol from ternary IPA–Methanol–Water mixtures using DMSO as an entrainer. In the present work, a three-column extractive distillation system was investigated for efficient separation of methanol, recovery of high-purity IPA, and regeneration of the DMSO solvent. The study aims to evaluate the effectiveness of DMSO in improving separation efficiency and solvent recovery in a continuous extractive distillation process[7-8].

## Process Simulation

The simulation is carried out using SCDS distillation model from the CHEMCAD simulator.

Following are the feed conditions considered for simulation

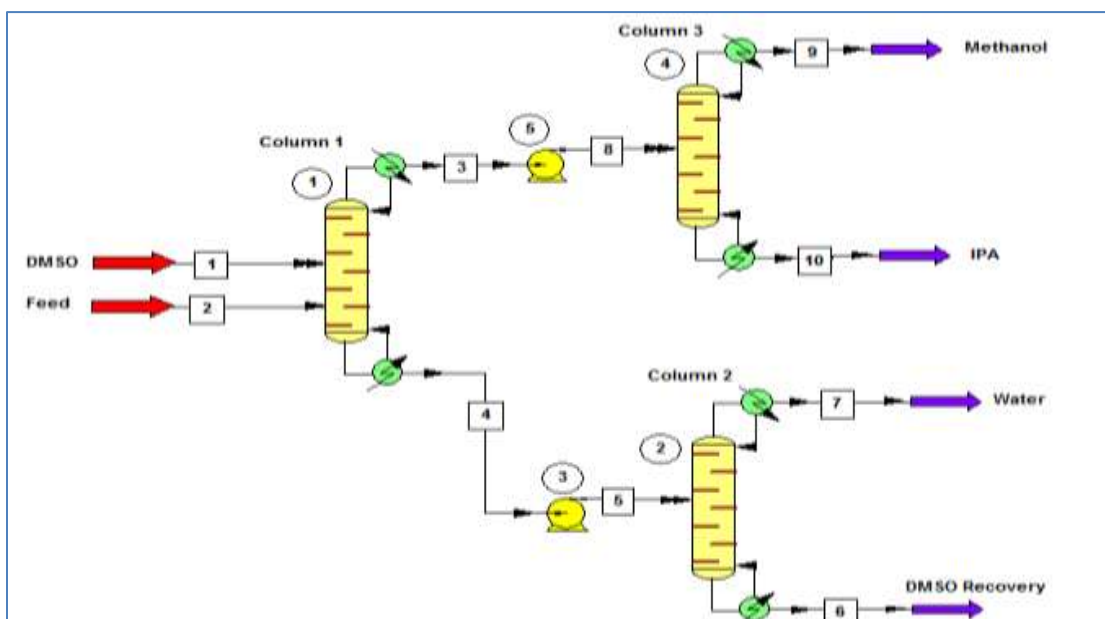
Temperature : 25 degree C

Pressure : 3.5 bar

Total feed flow : 1000 kg/hr

Composition of feed stream

IPA- 40% (by wt), Methanol - 40% (by wt), Water - 20% (by wt)



**Fig 1:** Three column Simulation of IPA-Methanol-Water

For a mixture comprising isopropanol (IPA), methanol, water, and dimethyl sulfoxide (DMSO), this study simulates a distillation-based separation procedure. High-purity IPA and methanol recovery from a feed mixture is the aim [8]. In the first column, the feed mixture was contacted with DMSO. The role of DMSO was to selectively retain water and methanol in the liquid phase, thereby improving the relative volatility between IPA and methanol[1-2]. The overhead product from Column 1 mainly contained IPA and methanol with very low water concentration, while the bottom product contained DMSO and water.

The bottom stream from Column 1 was sent to Column 2 for recovery of DMSO and removal of water. The results show excellent DMSO recovery with negligible solvent losses. The recovered solvent can be recycled back to the extractive distillation column, improving the economic feasibility of the process [1,4].

The overhead stream from Column 1 was fed to Column 3 for final separation of methanol and IPA. Column 3 successfully separated methanol and IPA into high-purity streams. The overhead temperature of methanol was approximately 64.2°C, which is close to the normal boiling point of methanol. Similarly, the IPA-rich bottom stream temperature was approximately 82°C, matching the boiling characteristics of IPA. These temperature profiles validate the effectiveness of the separation process[1,5,8].

**Result and Discussion:**

Below table shows the total stream summary of the three column

**Table 1:** Stream Summary

Stream No.	1	2	3	4	5	6	7	8	9	10
Stream Name	DMSO	Feed				DMSO Rec.	Water		Methanol	IPA
Temp C	25	25	69.809	124.5299	124.6817	188.2749	99.5839	69.9803	64.2174	81.9745
Pres bar	3.5	3.5	1	1	3.5	1	1	3.5	1	1



Enth kcal/h	- 5.6E+ 05	- 1.9E+ 06	- 1.2E+ 06	- 1.26E+ 06	- 1.3E+ 06	- 5.02E+05	- 7.2E+ 05	- 1.2E+ 06	- 7.06E+ 05	- 4.9E+ 05
Vapor mass frac.	0	0	0	0.0005878	0	0.00028762	0.15846	0	0	0
Total kmol/h	8.9589	30.2415	19.2051	19.9952	19.9952	8.9624	11.0328	19.2051	12.5284	6.6767
Total kg/h	700	1000.000	801.147	898.8532	898.8532	700.0463	198.8068	801.147	402.5334	398.6135
Total std L m3/h	0.6339	1.2036	1.0047	0.8328	0.8328	0.6339	0.1988	1.0047	0.5028	0.5019
Total std V m3/h	200.8	677.82	430.46	448.17	448.17	200.88	247.28	430.46	280.81	149.65
Component mass %										
Isopropanol	0	40.0000	49.9284	0.0000	0.0000	0.0000	0.0002	49.9284	0.6885	99.6525
Methanol	0	40.0000	49.9172	0.0100	0.0100	0.0000	0.0452	49.9172	99.2493	0.1000
Water	0	20.0000	0.1534	22.1138	22.1138	0.0100	99.9467	0.1534	0.0622	0.2455
DiMth Sulfoxide	100	0.0000	0.0010	77.8761	77.8761	99.9900	0.0079	0.0010	0.0000	0.0020

The simulation results demonstrate that extractive distillation using DMSO significantly enhances the separation efficiency of the IPA–Methanol–Water system. The process achieved:

- High-purity methanol recovery,
- High-purity IPA production,
- Nearly complete DMSO recovery.

The presence of DMSO altered the vapor–liquid equilibrium behavior of the system and enabled efficient separation of methanol and IPA, which is otherwise difficult using conventional distillation methods.

The material balance across the process was also found to be satisfactory. The total input flow rate of approximately 1700 kg/h was balanced by the output streams consisting of methanol, IPA, water, and recovered DMSO. Solvent losses were negligible, indicating stable operation and process reliability.

The process also demonstrated good thermal behavior. Methanol was recovered at lower temperatures due to its lower boiling point, whereas DMSO recovery occurred at significantly higher temperatures owing to its high boiling nature.



## Conclusion:

The present simulation study confirms that extractive distillation using DMSO is an efficient technique for the separation of IPA–Methanol–Water mixtures. The process successfully achieved:

- Methanol purity of 99.25 wt.%,
- IPA purity of 99.65 wt.%,
- DMSO recovery of approximately 99.99 wt.%.

The extractive distillation system effectively overcame the limitations of conventional distillation by modifying the relative volatility of the components. Minimal solvent loss and high product purity make the process economically attractive and suitable for industrial-scale applications. Therefore, DMSO can be considered an excellent entrainer for the separation and recovery of IPA and methanol from complex ternary mixtures.

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