RASĀYAN *J. Chem.*
Vol. 18 | No. 3 |1744-1752| July-September | 2025
ISSN: 0974-1496 | e-ISSN: 0976-0083 | CODEN: RJCABP
http://www.rasayanjournal.com
http://www.rasayanjournal.co.in

ENERGY EFFICIENT REACTIVE DISTILLATION SYNTHESIS OF N-HEXYL ACETATE: SIMULATION STUDY

Derick Rodrigues[1], Sunita Patil[2], Sharda Gadale[3] and Shambala Gadekar Shinde[1,✉]

[1]Department of Chemical Engineering, Bharati Vidyapeeth (Deemed to be University) College of Engineering, Pune 411043, India

[2]Department of Chemical Engineering, School of Engineering Management and Research, D Y Patil International University, Akurdi, Pune 411035, India.

[3]Yashwantrao Mohite College of Arts, Science and Commerce, Bharati Vidyapeeth (Deemed to be University), Pune 411038 India

✉Corresponding author: snshinde@bvucoep.edu.in

ABSTRACT

Synthesis of N Hexyl acetate by reactive distillation using toluene entrainer is proposed in this work. The key objective is to minimize the energy requirement of the classical reactive distillation method used for hexyl acetate synthesis. Adding toluene as an entrainer reduces the energy demand, leading to cleaner and more affordable energy consumption. Simulation is performed using the RADFRAC equilibrium stage model, and the required experimental data are extracted from the literature to establish the simulation base case. The thermodynamic model NRTL represents the non-ideal behavior of the system. Simulation results closely matched the experimental findings, and the validated model is used further to evaluate the system's performance with toluene as an entrainer. Parameters, reboiler duty, and entrainer flow rate are studied for minimizing energy requirement and quantitative conversion. A tremendous reduction in reboiler duty (50%) for the same operating conditions confirms that toluene entrainer is feasible for the continuous synthesis of hexyl acetate. This study significantly contributes to the use of alternative processes with affordable energy for cost reduction and making it potentially viable to the industry. 99.99 % conversion achieved ensures the successful application of this system in actual practice.

Keywords: Hexyl acetate, Reactive distillation, RADFRAC, Toluene, Entrainer, Energy Efficient.

RASĀYAN *J. Chem.*, Vol. 18, No. 3, 2025

INTRODUCTION

N-Hexyl Acetate, a nature-identical flavoring ingredient, is utilized in the food and perfume industry on a large scale, and its global production is estimated to be 1000 tons each year.[1,2] It is a highly versatile and stable ingredient, weaving its magic from the most exquisite fine fragrances to the everyday personal care items, and even, surprisingly, into a range of food flavorings due to its high miscibility with other solvents. The intricate thermodynamics and resemblance to other esterification systems motivate the industry partners to study the synthesis of n-hexyl acetate using different methods of synthesis. Literature witnesses' scarce study on the continuous synthesis of this acetate by the synthetic method. Continuous synthesis with different catalytic packing in a reactive distillation (RD) column was initiated by Schmitt *et al.,* 2004.[3] This study reflected the resemblance of the acetate with other acetates in series. Later, some investigations were made by modifying the catalytic internals in the same column to improve the conversion level.[4] A recent study reported the co-production of butyl and hexyl acetate with the advent of hexanol as an entrainer in both esterification reactions.[5] Research is done on the application of different catalysts like mesoporous MnO_2/C composite, vanadium pentoxide supported on alumina as a heterogeneous catalyst, for hexyl acetate synthesis, yet RD is rarely applied as a synthesis route for these studies.[6,7] RD is the intensified technology offering a transformative leap toward cleaner, more energy-efficient chemical processing, thus making it an important element toward the Sustainable Development Goal. It combines the benefits of chemical reaction and distillation in a single operation, thereby successfully applied to reversible chemical reactions wherein reaction equilibrium favors reactant conversion. Following are the primary benefits of combining reaction and distillation in a single unit: (1) By using Le Chatelier's principle, integrated

http://doi.org/10.31788/RJC.2025.1839321

separation of the products increases conversion (2) suppression of unwanted side reactions, resulting in a higher selectivity; (3) high conversion is possible at stoichiometric feed flow rates; and (4) heat of reaction is utilized for separation, avoiding hot spot problems. The reduced capital investment, lower energy consumption, and greater product yields enable reactive distillation to be an appealing alternative to the traditional method of synthesis.[8,9] Reactive distillation models accurately reflect integrated changes because of phase and chemical equilibria persisting in the column. Though the column must account for the hydrodynamics in the structured packings, it is challenging in actual practice, especially when the models are employed for various scales and operational situations. Though it is a proven synthesis tool explored for many esterification reactions to intensify the process, it is integrated with many intensifying tools to enhance the process. Recent studies reflect the use of decanter, side reactor, heat integration, pressure swing, heat pump, entrainer, and many other possible combinations in RD utilized to achieve cleaner products and byproducts, reduce carbon emissions, minimize energy, and enhance conversion.[10-15] These objectives directly relate to the sustainable development goals like clean and affordable energy, economic growth and industry, and innovations. Previous studies on n-hexyl acetate synthesis by RD reflect 93 % conversion, impure product purity, and elevated temperature profile in the column.[3,4] The experimental results depicted the successful applicability of RD as a route of synthesis, yet were deprived of intensified results such as quantitative conversion, product purity, and column stability. Surprisingly, we could rarely find any RD studies for hexyl ester, suggesting improvement in the conversion level and product purity using RD with entrainer as a route of synthesis. The system under study consists of three heterogeneous azeotropes between hexanol, hexyl acetate, and water, prevailing at nearby boiling temperatures of 97 °C. There is every chance of hexanol being carried in the distillate phase of the RD column and bringing conversion down. Also, the energy requirement of the process seems to be high, as the azeotrope temperatures are also high. This motivated us to examine the hexyl acetate synthesis by adding an entrainer, which forms an azeotrope with water at a much lower boiling point than that with hexanol and hexyl acetate. Toluene-water heterogeneous azeotrope, having a boiling point of 84 °C, is found suitable entrainer after preliminary study. This work aims to propose an optimized solution for the synthesis of hexyl acetate with quantitative conversion and minimum energy requirement. An alternate affordable energy route considering toluene as an entrainer in the RD system is investigated for identical column conditions. The process is further intensified for quantitative conversion and purity by optimizing the reboiler duty parameter. This study provides information on the efficient use of toluene entrainer for hexyl acetate synthesis and achieving 99.9% conversion with nearly half of the energy requirement compared to that of synthesis without using toluene. This encourages, production of intensified hexyl acetate on an industrial scale.

EXPERIMENTAL

Simulation Study

A base case simulation is established with experimental data from the literature, and the model is validated for further parameter study. The experimentally validated model is used to optimize reboiler duty for maximum conversion. The process is further assessed for a feasible entrainer with the help of the residue curve map (RCM), and toluene is selected for further energy optimization of the process without hampering quantitative conversion.

Base Case Parameters

The classical continuous RD column considered for study is divided into three sections, *viz* a reactive section with catalytic packings at the middle of the column, a stripping and a rectifying section at the bottom and top of the column, respectively. The feed streams are introduced in the reactive section counter. Currently, hexanol (Feed 1) and acetic acid (Feed 2) are supplied at the upper and lower ends of the reactive section, respectively. A simulation model to produce N-hexyl acetate is developed using the experimental information provided in the literature by Markus Schmitt.[3] N-hexanol (Feed 1) and acetic acid (Feed 2) are fed to the upper and lower ends of the reactant section, respectively, resulting in a counter-current flow of reactants in the column. The reflux is fed to the top of the reaction section. N-hexyl acetate is separated from n-hexanol in the stripping section and withdrawn as a bottom product. At the top of the column, phase separation occurs on condensation due to the heterogeneous azeotropic behavior of the mixture. The temperature profile in the rectifying section is found to be overheated by about 20 K, as reported in the

literature. The information extracted from experimental runs is used to build a simulation base case in Aspen version 14 and is depicted in Table-1.

Table-1: Reactive Distillation Hardware Parameters used for Base Case Radfrac Simulation

Parameter	Pilot-scale measurements	Parameter	Pilot-scale Measurements
Rectifying section		Stripping Section	
Height h / m	2.1	Height h / m	3.2
NTSM / (1/m)	3	NTSM / (1/m)	3
Rectifying Stages	6	Stripping Stages	9
Reactive section			
Height h / m	6.1	Thermodynamic Model	NRTL
NTSM / (1/m)	1		
Reactive Stages	6		
Catalyst amount mkat, W/kg	19.44		

Kinetic Model and Phase Equilibrium

The system 1 hexanol + water + acetic acid + hexyl acetate is a heterogeneous system with a wide immiscibility region. The presence of heterogeneous azeotropes and dimerization of acetic acid in the gas phase is characteristic of complexity and strong non-ideal behavior in the column. The kinetic data are referred to from the Schmitt paper and presented in Table-2.

Table-2: Kinetic Data Extracted from Literature[3]

K_1 (T °) (mol/s * mol_{H+})	K_{-1} (T°)(mol/s * mol_{H+})	E_1 (J/mol)	E_{-1} (J/mol)
0.02219	0.000695	34350	34350

Residue Curve Map (RCM) of Hexanol, Water, and Hexyl Acetate

The RCM for one hexanol-water-hexyl acetate is displayed in Fig.-1, and the azeotropic temperatures and compositions are exhibited in Table-3. The boiling temperatures of pure component hexanol, water, and hexyl acetate are 157.2 ºC, 100 ºC, and 171.3 ºC, respectively. In the system, two heterogeneous azeotropes, namely acetate-water (97.64 ºC) and alcohol-water (97.88 ºC), and a ternary heterogeneous azeotrope involving acetate-hexanol-water (97.63 ºC) coexist with almost similar boiling points. This further complicates the separation process, the ternary azeotrope being the lowest boiling azeotrope among the three hetero azeotropes carries some amount of hexanol to the decanter and poses a challenge for column operation and making the separation more difficult. Due to the liquid splits across the top stages in the rectification zone of the RD column, alcohol is undoubtedly carried in the decanter and is a significant reason for the impure water purity and decrease in conversion. This distribution has the potential to transport alcohol to the decanter and be lost in the aqueous phase, though some percentage can be subsequently recycled as part of the organic phase. The interaction parameters used are extracted from the Aspen database and are reported in Table-4.

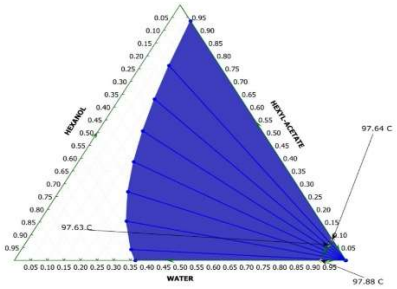


Fig.-1: Residue Curve Map for Hexyl Acetate/ Hexanol /Water System

Table-3: Azeotropic Composition and Temperature of 1 Hexanol/Water/Hexyl Acetate

S. No.	Heterogeneous Azeotrope	Composition		Temperature ºC
		Mole Basis	Mass Basis	
1.	Hexanol	0.0754	0.3162	97.88
	Water	0.9246	0.6838	

2.	Water	0.9182	0.5836	97.64
	Hexyl Acetate	0.0818	0.4164	
3.	Hexanol	0.0216	0.0802	97.63
	Water	0.9172	0.5996	
	Hexyl Acetate	0.0612	0.3202	

Table-4: Binary Interaction Parameters Extracted from the Aspen Database

Component i	water	water	water	acetic acid
Component j	n-hexyl acetate	n-hexanol	acetic acid	n-hexanol
a_{ij}	9.3181	2.9892	3.3293	0.0
a_{ji}	0.3504	0.1128	-1.9763	0.0
b_{ij}	-320.4472	949.2321	-723.8881	-211.3257
b_{ji}	413.7759	202.5458	609.8886	816.9305
$\alpha_{ij} = \alpha_{ji}$	0.2	0.32	0.3	0.3

Comparison of Base Case with Experimental Results

In a simulation case, it is important to evaluate the accuracy and reliability of the simulation results. In this study, the simulation results were found to match the base (experimental) results reported in literature,[3] quite prominently. This means that the simulation accurately replicated the real-world scenario being modeled, and the results were consistent with what was expected based on prior knowledge. Matching the base results is a significant achievement in simulation studies, as it validates the simulation methodology and helps to build confidence in the results. It also means that the simulation can be used to make predictions about similar scenarios in the future, with a high degree of confidence in the accuracy of the results. For a feed flow rate of 0.05 kmol/hr, a total of 22 stages and reactive stages 7, the conversion achieved was 99 %, which is close to literature data (93%) for identical column conditions. Figure-2 displays the simulated results.

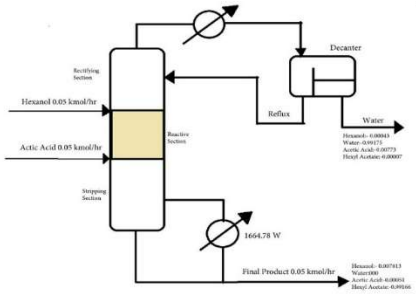


Fig.-2: Schematic Diagram for Base Case Hexyl Acetate Synthesis. Column Conditions: Number of Stages = 22; Feed Flow Rate of Acetic Acid and Hexanol = 0.050 kmol/h each; Number of Reactive Stages, 11-17; Reboiler Duty = 1664.78 W; Conversion = 99.17%

Reboiler Duty Optimization

Reboiler duty optimization is necessary to minimize the energy requirement of the process. This parameter was studied after successfully validating the simulator; the same base case was utilized for studying the effect of reboiler duty, for further optimizing the process. The effect of reboiler duty (900 to 2000 Watts) on conversion was thoroughly explored. The findings unambiguously show that reboiler duty and system conversion are related clearly and directly (Fig.-3). It was noted that the conversion of hexanol constantly displayed an increasing trend as the reboiler duty increased, leading to improved conversion efficiencies. Notably, the study also determined a critical threshold, requiring a reboiler duty of around 1600 Watts, for attaining a 99% conversion of hexanol in the system.

A crucial factor examined at various reboiler duties was the temperature profile of the distillation column. A noteworthy finding was that the temperature profiles of the column varied for each reboiler duty (Fig.-4).

It is necessary to maintain the temperature profile of the column below the thermal stability limit of the catalyst. In general, the widely used ion exchange catalyst is stable up to 130 °C. The reboiler duty study helps us to identify the feasible operating range to satisfy the column performance. It is observed that a reboiler duty of 2000 watts resulted in attaining the temperature profile of the reactive stage from 91 to 99

°C. An intriguing finding of the study was that though the mean temperature of the reactive stage (stages 10-16) exhibited an increasing trend with the reboiler duty, the preferred temperature ranges of 91 to 97°C in the reactive section revealed a stable zone. It is crucial to maintain a constant temperature within this range since the catalyst may become permanently damaged at temperatures beyond the thermal stability limit.

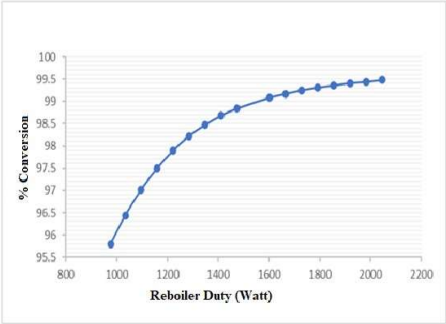


Fig.-3: Conversion of n-hexanol at Reboiler Duty 1000-2200 Watts

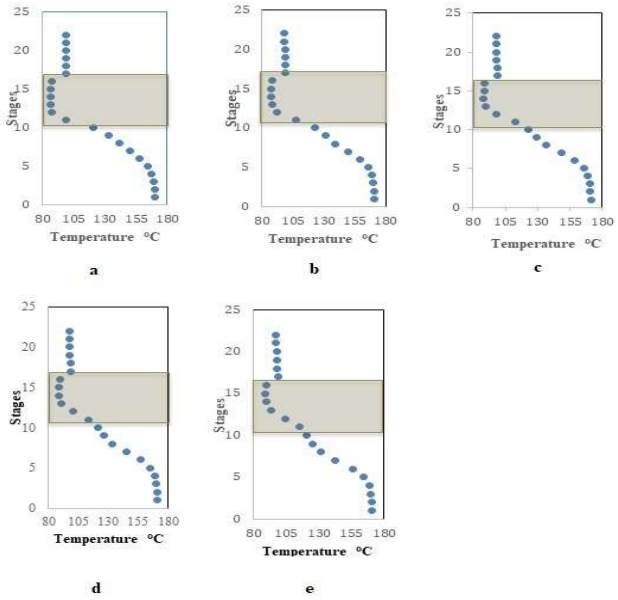


Fig.-4: Temperature Profile of Reactive Distillation Column at different Reboiler Duty (a) 1000W, (b) 1250W, (c) 1500W, (d) 1750W, (e) 2000W

Entrainer Enhanced Reactive Distillation

Application of an entrainer concurrently improves the internal alcohol recycling by forming an azeotrope with water at a lower temperature and improves the separation of end streams. Many esterification systems have demonstrated improved conversion by adding an entrainer to the system.[16-19] Entrainer plays a soothing role in maintaining the thermal stability of the column and suppresses the undesired azeotrope formation in the column.[20,21,22] The added advantage of adding an entrainer is in reducing the reboiler load of the column. The wise selection of the entrainer completely depends upon the thermodynamic behavior of the selected entrainer with the components of the system and the azeotropic temperature. Toluene and epichlorohydrin were initially screened for simulation studies.

Residue Curve Maps for Toluene and Epichlorohydrin as Entrainers

RCM of Toluene

The current system consists of four heterogeneous azeotropes: acetate-water, alcohol-water, toluene-water, and acetate-alcohol-water. Among these, the acetate-water and alcohol-water azeotropes exhibit similar boiling temperatures, while the acetate-alcohol-water azeotrope is a minimum boiling ternary azeotrope at

97.63 ºC (Fig.-1). It is important to highlight that when toluene is added to the system, the toluene-water azeotrope possesses the lowest boiling point among all the azeotropes present in the system (84.4 ºC). The identification of the lowest boiling azeotrope holds significant importance in the design of an efficient separation process, as it enables the simplification of separation operations and reduces the energy requirements. Moreover, the presence of multiple heterogeneous azeotropes with closely matched boiling points introduces complexities in the separation process. Careful considerations are necessary in selecting appropriate separation techniques capable of effectively separating these complex mixtures. The RCM for the acetate-water-toluene system (Fig.-5) reflects that most of the ternary map is covered with a heterogeneous region. Toluene advantageously forms an azeotrope only with water and not with alcohol or acetate, which makes it a potential entrainer for many RD synthesis studies.[23,24,25]

RCM of Epichlorohydrin

Epichlorohydrin was checked for the feasibility of the present system under consideration. Three different hetero azeotropes are persisting in the ternary mixture. The binary azeotrope of water-epichlorohydrin (96.72 ºC), water-hexanol (97.98 ºC), and the ternary azeotrope of hexanol-water-epichlorohydrin (96.43ºC °C), all have close boiling temperatures and hence possess difficulty in separation.

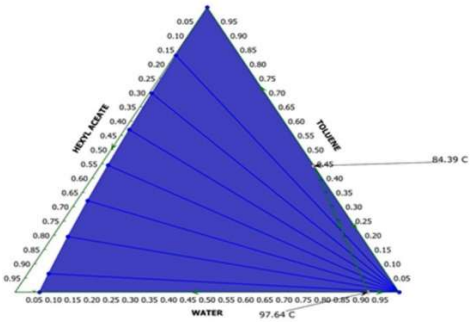


Fig.-5: Residue Curve Map for Hexyl Acetate/ Toluene /Water System

The separation process is complicated and intricated by the occurrence of three heterogeneous azeotropes with comparable boiling temperatures when epichlorohydrin is selected as entrainer. It is difficult to produce good separation since the boiling points of all the azeotropes are at a minute difference. To get around these issues and reach the appropriate level of purity for each component, additional separation techniques or innovative process designs must be considered. RCM for the system (Fig.-6) visibly indicates low heterogeneity in the distillate, and hence, for hexyl acetate synthesis, this is undesired as all the azeotrope temperatures are hardly at one degree difference. Compared with toluene and epichlorohydrin, toluene was found to be more feasible for this system as it ensures a large heterogeneity envelope with a wide gap between the azeotropic temperature of the components.

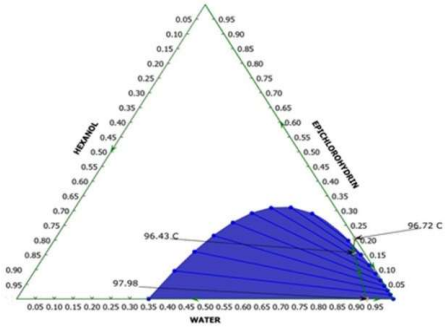


Fig.-6: Residue Curve Map for Hexanol/ Epichlorohydrin /Water System

Simulation of Entrainer-Based Reactive Distillation

The toluene-water azeotrope has the lowest boiling heterogeneous azeotrope in the current system, with a boiling point of 84.39 °C. Because of this property, toluene is an excellent entrainer in the reactive distillation system used in the production of n-hexyl acetate. Toluene is used in a reactive distillation

process to adjust the azeotropic behavior of the system and improve product separation. It serves as a selective solvent, shifting the azeotropic composition and modifying the boiling temperatures of the constituents due to the presence of low low-boiling azeotropic mixture. Selective solvent qualities enable n-hexyl acetate extraction more easily, resulting in higher product purity and yield. Continuous synthesis of n-hexyl acetate by RD can produce effective separation and improved process performance by utilizing the toluene-water azeotrope as an entrainer.

To assess the purity and conversion of n-hexyl acetate, a simulation environment based on Aspen Plus V14 was created, wherein toluene was used as an entrainer. The simulation findings demonstrated beneficial effects, both in energy savings and process performance. Investigations and tuning of parameters were done to identify the optimal set of conditions. The favorable results show that the developed method is more efficient and effective in the synthesis of n-hexyl acetate. The energy reductions generated through simulation highlight the potential for resource conservation and cost reduction in the process's industrial-scale deployment.

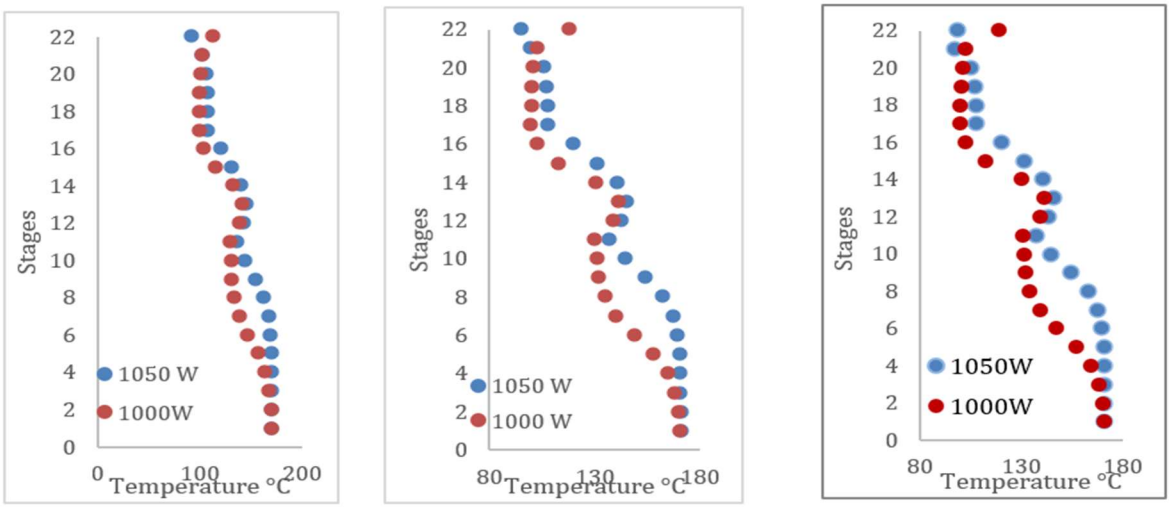
RESULTS AND DISCUSSION

Synthesis of hexyl acetate using toluene entrainer was studied by varying entrainer flow rate and reboiler duty to optimize the column performance. The same RADFRAC model (total 22 stages) was used for entrainer study, with the introduction of toluene just above the reactive section. The feed mole ratio of alcohol and acid was kept at one and introduced in the middle of the reactive section. The conversion rates were assessed at two different reboiler duties (1000 and 1050 watts) and three alternative flow rates of toluene (0.0001, 0.0002, and 0.0003 kmol/hr). Notably, the study's focus was on hexanol conversion, which consistently achieved quantitative 99% conversion across all measured toluene flow rates. Surprisingly, the data revealed an important finding on the system's reboiler duty. The application of entrainer resulted in a significant reduction in the required reboiler duty to achieve quantitative conversion (99%) as compared to the reactive distillation system without an entrainer (Table-5). Reboiler duty was reduced to fifty percent, due to the presence of toluene water azeotrope, which shifted the equilibrium and enhanced the conversion. The soothing effect of toluene demands less energy for improved process performance. In the case of without toluene-free system, it is observed that 99.6 % conversion is achieved with a reboiler duty above 2000 W, whereas comparable conversion is achieved in the case of with toluene system for a 1000 W reboiler duty requirement. These results draw attention to the system's potential for energy savings since lower reboiler duty suggests improved performance with an affordable energy requirement of the system.

In addition to reboiler duty and conversion rates, the temperature profile of the column was scrutinized for process optimization. The simulation results exhibited that the temperature profile stayed within the typical range of catalyst stability, preserving the catalyst's integrity and efficiency. This finding is particularly important since it assures the catalyst's durability and peak performance, which are essential for sustaining steady and high conversion rates. This stability is further demonstrated graphically (Fig.-7), which offers insightful information about the thermal behavior of the system and confirms that the operating parameters are suitable for the catalyst's prolonged activity. For entrainer flow rate 0.001 to 0.003 kmol/hr, the temperature of the column varies from 100 to 140 °C for the reactive stages, where toluene-water azeotrope plays a significant role in shifting the equilibrium towards the right. Water, as soon as formed, is directed to the distillate, and this favors the forward reaction. Though the simulation studies were performed with available kinetics from the literature, it is quite visible that the catalyst's sustainability to a temperature range below 150 °C is feasible for the reaction. Widely used ion exchange resins having thermal stability up to 170 °C can be used for the continuous synthesis of this ester.

Table-5: Effect of Entrainer Flow Rate and Reboiler Duty on Conversion

Entrainer Flow Rate (kmol/hr)	Reboiler Duty (Watt)	Conversion of n-hexanol (%)
0.0001	1000	99.67
	1050	99.99102
0.0002	1000	99.72
	1050	99.99166
0.0003	1000	99.66
	1050	99.99174



(a) (b) (c)

Fig.-7: Temperature Profile of Reactive Distillation Column with 1:1 Hexanol: Acetic Acid Feed Mole Ratio; Reboiler Duty 1000 and 1050 W and at different Entrainer Flow Rate a) 0.0001 kmol/hr, b) 0.0002 kmol/hr, and c) 0.0003 kmol/hr. Overall, the Objective of this Study is to Assess the Feasibility of Toluene as an Entrainer for the Synthesis of N-hexyl acetate and reduce the Energy Requirement of the RD Process, Demonstrating that Quantitative Conversion is Satisfied

CONCLUSION

Synthesis of n-hexyl acetate using toluene entrainer in the RD system is explored in this work. An experimentally validated simulator is used to study and optimize the process parameters. Entrainer flow rate and reboiler duty were altered and assessed for achieving quantitative conversion. The addition of entrainer toluene to the system reduced the reboiler duty by fifty percent, with 99.9 % conversion in all observations. This indicates energy requirements of the system can be reduced to nearly half by adding toluene to the system. This study suggests that continuous synthesis of n-hexyl acetate with toluene as an entrainer can enhance the performance of the RD column in actual practice and achieve the sustainable development goal of clean and affordable energy in the process Industry.

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

AUTHOR CONTRIBUTIONS

The present work is related to *SDG-7: Affordable and Clean Energy*. All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

Derick Rodrigues https://orcid.org/0009-0009-0173-2135
Sunita Patil https://orcid.org/0000-0002-9709-1927
Sharda Gadale https://orcid.org/0000-0002-2872-505X
Shambala Gadekar Shinde https://orcid.org/0000-0001-7090-4097

REFERENCES

1. N.T.C. Duong, A. Uthairatanakij, N. Laohakunjit, P. Jitareerat and N. Kaisangsri, *Food Bioscience*, **52**, 102410(2023), https://doi.org/10.1016/j.fbio.2023.102410
2. E.G. Dennis, R.A. Keyzers, C.M. Kalua, S.M. Maffei, E.L. Nicholson and P.K. Boss, *Journal of Agriculture and Food Chemistry*, **60(10)**, 2638(2012), https://doi.org/10.1021/jf2042517

3. M. Schmitt, H. Hasse, K. Althaus, H. Schoenmakers, L. Gotze and P. Moritz, *Chemical Engineering and Processing: Process Intensification*, **43(3)**, 397(2004), https://doi.org/10.1016/S0255-2701(03)00124-7
4. M. Schmitt, C. von Scala, P. Moritz and H. Hasse, *Chemical Engineering and Processing: Process Intensification*, **44(6)**, 677(2005), https://doi.org/10.1016/j.cep.2003.07.005
5. K. Namgung, H. Lee, W. Jang, H. Mo and J. W. Lee, *Chemical Engineering and Processing: Process Intensification*, **154**, 108048(2020), https://doi.org/10.1016/j.cep.2020.108048
6. Z. Yang, Y. Pan, Z. Mei and W. Zhang, *Applied Surface Science*, **258(10)**, 4756(2012), https://doi.org/10.1016/j.apsusc.2012.01.079
7. V. S. Patil and P. R. Gogate, *Chemical Engineering Journal*, **289**, 513(2016), https://doi.org/10.1016/j.cej.2016.01.015
8. I. Pazmino-Mayorga, M. Jobson and A. A. Kiss, *Industrial & Engineering Chemistry Research*, **62(14)**, 5907(2023), https://doi.org/10.1021/acs.iecr.2c04540
9. D. Liu, Z. Lin, W. An, R. An and H. Bie, *Chemical Engineering and Processing-Process Intensification*, **153,** 107930(2020), https://doi.org/10.1016/j.cep.2020.107930
10. A-E. Plesu Popescu, J. Bonet, and J. Llorens, *Energy & Environment*, **32(8)**, 1457(2020), https://doi.org/10.1177/0958305X20937689
11. Y. Hu, L. Wang, J. Lu, L. Ding, G. Zhang, Z. Zhang, J. Tang, M. Cui, X. Chen and X. Qiao, *ACS Omega,* **8(14),** 13192(2023), https://doi.org/10.1021/acsomega.3c00469
12. X. Gao, Y. Yang, M. Chen, Q. Cheng and K. Lu, *Separation and Purification Technology*, **300,** 121755(2022), https://doi.org/10.1016/j.seppur.2022.121755
13. X. Geng, H. Zhou, P. Yan, H. Li, X. Li and X. Gao, *Process Safety and Environmental Protection,* **158**, 525(2022), https://doi.org/10.1016/j.psep.2021.12.029
14. B. Sulgan, P. Furda and Z. Labovska. *Chemical Engineering Journal*, **471,** 144298(2023), https://doi.org/10.1016/j.cej.2023.144298
15. T.W. Wu and I.L. Chien, *Separation and Purification Technology*, **294,** 121159(2022), https://doi.org/10.1016/j.seppur.2022.121159
16. M. Cho, and M. Han, *Journal of Process Control,* **61**, 58(2018), https://doi.org/10.1016/j.jprocont.2017.11.011
17. M. Cho, S. Jo, G. Kim and M. Han, *Industrial & Engineering Chemistry Research,* **53(19)**, 8095(2014), https://doi.org/10.1021/ie403049z
18. G. N. Patil and N. Gnanasundaram, *ECS Transactions*, **107**, 9841(2022), https://doi.org/10.1149/10701.9841ecst
19. K. Namgung, H. Lee, W. Jang, H. Mo and J.W. Lee, *Chemical Engineering and Processing: Process Intensification*, **154,** 108048(2020), https://doi.org/10.1016/j.cep.2020.108048
20. H. Xia, X. Dai, Q. Ye, S. Feng, R. Li and X. Suo, *Computers & Chemical Engineering,* **106**, 559(2017), https://doi.org/10.1016/j.compchemeng.2017.08.003
21. Z.Y. Kong, G.C. Zarazua, H.Y. Lee, J. Chua, J. G. Segovia-Hernandez and J. Sunarso, *Process Safety and Environmental Protection,* **166,** 574(2022), https://doi.org/10.1016/j.psep.2022.08.056
22. Q. Wu, Z. Wang, B. Wang, W. Xu, J Ruan, R. Hu, J. Zhong, L. Xin, Z. Zhu, Y. Wang and P. Cui, *Process Safety and Environmental Protection,* **190,** 110(2024), https://doi.org/10.1016/j.psep.2024.07.035
23. S. Kale, S.B. Umbarkar, M.K. Dongare, R. Eckelt, U. Armbruster and A. Martin, *Applied Catalysis A: General*, **490,** 10(2015), https://doi.org/10.1016/j.apcata.2014.10.059
24. S. Gadekar-Shinde, B. Reddy, M. Khan, S. Chavan, D. Saini and S. Mahajani, *Industrial & Engineering Chemistry Research,* **56**, 832(2017), https://doi.org/10.1021/acs.iecr.6b03489
25. K. Jayant, C. Gupta, S. Seethamraju and S. M. Mahajani, *Separation and Purification Technology*, **331**, 125650 (2024), https://doi.org/10.1016/j.seppur.2023.125650

[RJC-9321/2025]