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Extractive Distillation of Acetone/Methanol Mixture Using Water as Entrainer

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The acetone—methanol extractive distillation using water as an entrainer was simulated on *Aspen Plus* software package using rigorous methods. Calculation of the vapor—liquid equilibrium for the ternary system was done by the UNIQUAC model according to the experimental results obtained in a previous work. The effects of the solvent to feed molar ratio, reflux ratio, feed stage, feed solvent stage, and solvent feed temperature were studied to obtain the best design of the extractive distillation column with minimal energy requirements. The most appropriate configuration is 52 theoretical stages. The best binary mixture and entrainer feeding stages were obtained at 48 and 22 respectively with a solvent to feed molar and reflux ratio of 2.0 and 5.0, respectively. The simulation results show the effect of the main variables on the extractive distillation process.

1. Introduction

Acetone and methanol are extensively used as solvents or reagents in organic chemistry. Additionally, acetone is a solvent frequently used in industry to dissolve plastics, like a drying agent, and it is the primary component in nail polish remover. Methanol is also a commonly used solvent, and its mixtures with acetone are usually observed, being necessary to separate these volatile solvents for future applications. Distillation is one of the major importance separation processes in chemical engineering in which the separation is reached because of the volatility difference of the components.¹

The recovering of volatile solvents with close boiling point or azeotropic systems is difficult by conventional distillation techniques. Advance techniques like pressure distillation, reactive distillation, and extractive distillation may be used to separate such mixtures. In the extractive distillation is required a third component, an entrainer, which modifies the relative volatility of the mixture components. The entrainer selection is an important step because the separation effectiveness depends on the interactions between this component and the azeotropic mixture.

The acetone-methanol system has a minimum boiling point azeotrope,³ and the extractive distillation is a possible method used to separate this azeotropic mixture. Many works have studied the vapor-liquid equilibrium of this system and suggest water as an entrainer. ⁴⁻⁷ The extractive distillation of this system had been reported widely in the literature 1,8-14 and some simulation studies of the process have been reported. ^{8,10,11} In this study, the extractive distillation of an acetone-methanol mixture, and the effect of the main variables on mixture separation, were studied by simulation on Aspen Plus 2006 software. The thermodynamic package using UNIQUAC model was used to evaluate the vapor-liquid equilibrium (VLE), according to the experimental data obtained by the authors in a previous work for the acetone-methanol-water mixture. The simulation was carried out taking into account pressure drops and heat-integration, in order to compare the results with those reported previously in literature in which the property estimation was done by other thermodynamic models that cannot represent accurately the VLE or considered simplifying assumptions.

2. Extractive Distillation

Extractive distillation is a separation process used to separate mixtures that are difficult or impossible to separate by conventional distillation. In extractive distillation, a third component (solvent or entrainer) is added to the binary mixture to increase the relative volatility of the original components.¹⁵

The process flow diagram of the extractive distillation process is presented on Figure 1. The process has two columns, one for extractive separation and another for solvent recuperation. The azeotropic mixture and the solvent are fed to the first column, in which the components boil separated allowing the less volatile components to collect in the bottoms and in the top of the column the light key component. The bottom product is fed to the second column in which the solvent is recovered and recycled to the extractive distillation column.

The entrainer must have special characteristics to achieve the desired separation as follows: thermal stability, low toxicity, higher boiling points, easily recovery, change the relative volatility between the key components, and selectivity. ^{16,17}

The design and analysis of the separation process and especially the distillation process involve the use of the residue curve maps. 18 These are tools that allow us to determine whether the entrainer is or is not the most effective to obtain the desired separation. The residue curve maps for extractive distillation are composed by a stable node that corresponds to the solvent vertex, an unstable node that corresponds to the azeotrope, and the saddle points located at the vertex of the azeotropic mixture. 18 Figure 2 presents the residue curve map for the acetone-methanol-water system. The azeotropic mixture of acetone (bp 56.14 °C) and methanol (bp 64.53 °C) presents a minimum boiling point at 55.24 °C and 1 atm. From Figure 2, it is observed that water is a feasible entrainer for the acetone-methanol separation because the residue curve map has the optimal configuration (stable and unstable nodes, and saddle points) for the extractive distillation.

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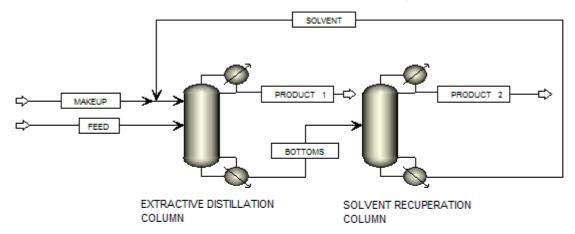


Figure 1. Extractive distillation process.

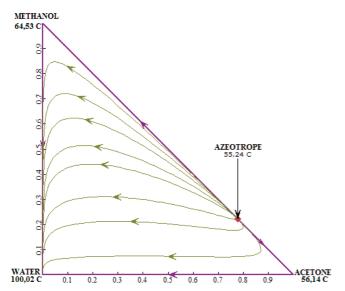


Figure 2. Residue curve map for acetone—methanol—water system at 1 atm calculated using the UNIQUAC model.

3. Simulation of the Acetone-Methanol Extractive Distillation Column

Previous to the simulation, the ternary vapor—liquid equilibrium (VLE) of the acetone—methanol—water system was determined experimentally. Briefly, mixtures of acetone—methanol with a close ratio to the azeotrope composition, and with different solvent to feed molar ratios, were prepared in a modified Othmer still. After the VLE was achieved (constant temperature throughout the system), samples of condensed vapor and liquid were taken for GC analysis. Each assay was made in duplicate. Figure 3 shows the pseudo-binary diagram obtained for a solvent to feed molar ratio (E/F) of 3.0.

Three thermodynamic models (Wilson, NRTL, and UNI-QUAC) were analyzed to determine which model is the most suitable to predict the system performance. The obtained results show that the UNIQUAC model presented the highest accuracy, a mean absolute error of 0.009 \pm 0.015 and 0.246 \pm 0.114 °C for the composition and temperature, respectively, whereas the obtained mean absolute error of composition and temperature were 0.012 \pm 0.015 and 0.417 \pm 0.190 °C for the Wilson model and 0.011 \pm 0.015 and 0.494 \pm 0.213 °C for NRTL model. Therefore, the UNIQUAC model was selected for the prediction of physical properties in the simulation.

To establish the operating conditions for the extractive distillation process, a sensitivity analysis was done. The design

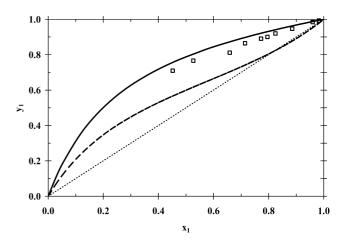


Figure 3. Pseudo-binary x-y plot for the acetone (1)—methanol (2) system with an entrainer to feed molar ratio 3. Solid and dashed lines predicted by UNIQUAC model for the pseudo-binary and binary systems, respectively.

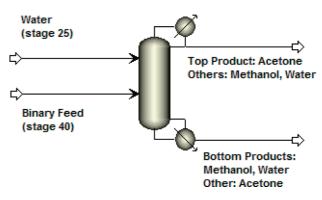


Figure 4. Process flow diagram for the extractive distillation column.

Table 1. Process Design Parameters

parameter		value
feed mole flow (kmol/h)		100
distillate mole flow (kmol/h)		76
feed temperature (°C)		20
mole fraction of binary feed	acetone	0.7775
	methanol	0.2225
pressure (atm)		1

of the extractive distillation column operation was taken from the Luyben⁸ work (Figure 4). The feed conditions of the azeotropic mixture and the entrainer are presented in Table 1.

3.1. Sensitivity Analysis Results. The parameters analyzed were as follows: number of stages (NS), reflux molar ratio (R),

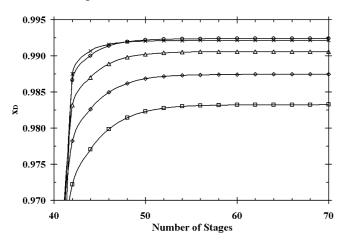


Figure 5. Number of stages and reflux ratio influence on the distillate acetone mole composition. Operational conditions: BFS 48, EFS 22, EFT 47 °C, and E/F 2.0. Evaluated refluxes: $3.0 \ (\times)$, $4.0 \ (o)$, $5.0 \ (\triangle)$, $6.0 \ (\diamondsuit)$, and $7.0 \ (\Box)$.

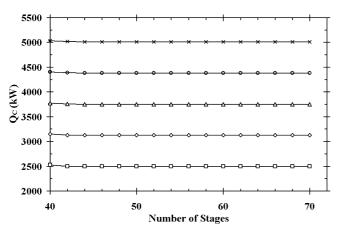


Figure 6. Number of stages and reflux ratio influence on the condenser duty. Operating conditions: BFS 48, EFS 22, EFT 47 °C, and E/F 2.0. Evaluated refluxes: $3.0 \ (\times)$, $4.0 \ (o)$, $5.0 \ (\triangle)$, $6.0 \ (\diamondsuit)$, and $7.0 \ (\Box)$.

binary feed stage (BFS), entrainer feed stage (EFS), entrainer feed temperature (EFT), and entrainer to feed molar ratio (E/F). The binary mixture was fed in the extractive distillation column at azeotropic composition.

Figure 5 shows the influence of the reflux ratio and the number of stages on the distillate mole composition (x_D) . According to the ASTM purity standard specification for acetone is 99.5% mass (~99.0% mol), this specification can be achieved using refluxes among 3.0 and 5.0. The highest x_D was obtained at a reflux of 4.0. It is observed that an increase of reflux causes a decrease in the distillate. This is because high reflux causes the dilution of the liquid phase, which should be rich in solvent. From Figure 5, is also possible to observe that with a number of stages greater than 52 the composition of the distillate does not change significantly. Results show that the column may have 52 stages and be operated at a reflux rate between 3.0 and 5.0.

The effect of reflux ratio and number of stages on the condenser (Q_C) and reboiler (Q_R) duties is presented in Figures 6 and 7, respectively. For both cases, duties did not change with the number of stages. Nevertheless, reflux rate had an important influence on the column energy consumption. Heating and cooling requirements presented a direct proportional relationship with the reflux ratio. From the sensitivity analysis, it is possible to conclude that at a reflux ratio of 5 the energy consumption and distillate composition requirements are satisfied.

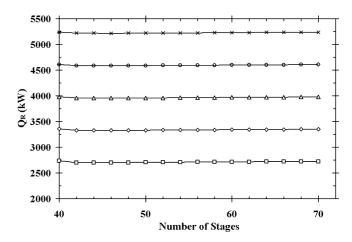


Figure 7. Number of stages and reflux ratio influence on the reboiler duty. Operating conditions: BFS 48, EFS 22, EFT 47 °C, and E/F 2.0. Evaluated refluxes: $3.0 \ (\times), 4.0 \ (o), 5.0 \ (\triangle), 6.0 \ (\diamondsuit), and 7.0 \ (\Box).$

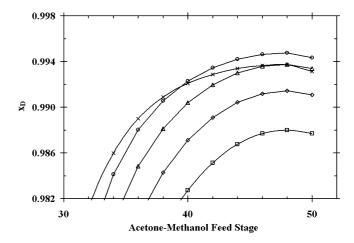


Figure 8. Binary feed stage and reflux ratio influence on the distillate acetone mole composition. Operating conditions: NS 52, EFS 22, EFT 47 °C, and E/F 2.0. Evaluated refluxes: $3.0 \ (\times), 4.0 \ (o), 5.0 \ (\Delta), 6.0 \ (\diamondsuit),$ and $7.0 \ (\Box).$

Figure 8 shows the results of the reflux ratio and the binary feed stage analysis. As can be seen, at reflux rates between 3.0 and 5.0 were obtained the greatest distillate compositions, with a difference among them no higher than 0.02. However, differences on distillate acetone mole composition at reflux ratios higher than 5.0 were around 0.10. The highest distillate acetone composition was reached when the binary mixture was fed between the 46 and 48 stages. Because of longer contact time between the azeotropic mixture and the solvent, higher purity in the distillate, the azeotropic mixture was fed near to the column bottoms.

Figure 9 presents the influence of the binary feed stage on the distillate composition and energy duty. From the above analysis, the reflux ratio was kept constant (5.0). At stages greater than 42, the condenser and reboiler duties and distillate composition did not change significantly (Figure 9). Hence, a feasible binary feed location is at stage 48 because the binary mixture—entrainer contact time is kept long. It is also possible to observe that reboiler duty was greater than condenser duty. The increased energy consumption is produced when the binary mixture is fed as a saturated liquid near to the reboiler. At stage 22, the reboiler and condenser duties decline; this is caused by the entrainer feeding.

The reflux ratio and the entrainer feed stage effect on distillate acetone composition are presented in Figure 10. It is noticed that the highest acetone compositions in the distillate were

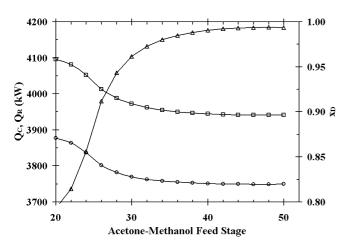


Figure 9. Binary feed stage effect on distillate composition (Δ) and energy duty (condenser \bigcirc , reboiler \square). Operating conditions: NS 52, EFS 25, EFT 47 °C, R 5.0, and E/F 2.0.

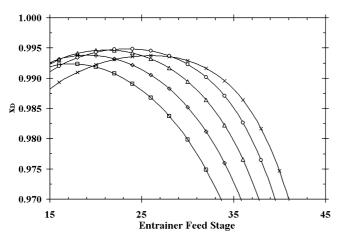


Figure 10. Entrainer feed stage and reflux ratio influence on the distillate acetone mole composition. Operating conditions: NS 52, BFS 48, EFT 47 °C, and E/F 2.0. Evaluated refluxes: $3.0 \ (\times)$, $4.0 \ (o)$, $5.0 \ (\Delta)$, $6.0 \ (\diamondsuit)$, and $7.0 \ (\square)$.

obtained at reflux ratios of 4.0 and 5.0, and that, at greater values of entrainer feed stage, acetone composition in the distillate was lower. This is due to the interaction between entrainer and azeotropic mixture components that occur predominantly in the liquid phase. When the solvent is fed in the top, it is possible to guarantee that the entrainer is present in the liquid phase in all of the stages below. From these results, at stage 22 was obtained the highest acetone concentration, and then this is a feasible stage to feed the solvent.

The energy consumption was less when the solvent was fed at stages near to the top of the column (Figure 11). This could be owed to the higher entrainer contact with the vapor phase that caused a higher methanol transferred to the liquid phase. Therefore, the flow to the reboiler is greater. If the solvent is fed near to the bottoms, a minimal quantity of methanol leaves the vapor phase so the flow to the condenser and the energy consumption increases. Binary mixture feeding caused an increase on reboiler and condenser duties. For that reason, in proximity to stage 48 an increase on reboiler and condenser duties was observed. The influence of the entrainer feed stage on the distillation composition showed that acetone composition in the distillate is higher with the decrease of the entrainer feed stage. At stage 22, the composition of the distillate had a maximum value. This result agrees with those results presented in Figure 10. As can be seen on Figure 12, at high reflux rates and E/F ratio the distillate acetone composition was greater.

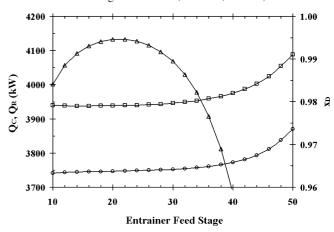


Figure 11. Entrainer feed stage effect on distillate composition (Δ), and energy duty (condenser \bigcirc , and reboiler \square). Operating conditions: NS 52, BFS 48, EFT 47 °C, R 5.0, and E/F 2.0.

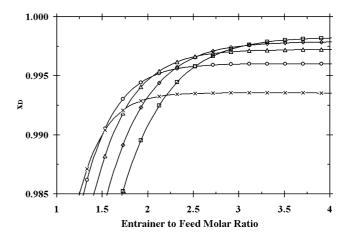


Figure 12. Entrainer to feed molar ratio and reflux ratio influence on the distillate acetone mole composition. Operating conditions: NS 52, BFS 48, EFS 22, and EFT 47 °C. Evaluated refluxes: 3.0 (\times), 4.0 (o), 5.0 (Δ), 6.0 (\diamondsuit), and 7.0 (\square).

Because of higher E/F ratios, the entrainer dilution caused by the reflux is small and the purity of distillate increases.

At entrainer to feed molar ratios of 2.5 or higher, the distillate composition remained constant (Figure 12). For all of the evaluated E/F range, the condenser duty remained constant. However, the reboiler duty presented significant changes with the increased E/F. This is associated with higher E/F values owing to larger liquid volumes needed for vaporization; therefore the energy consumption in the reboiler is increased. An optimal value could be 2.0 because with this value it was possible to obtain high acetone purity and lower energy consumptions (Figure 13). Also, a rise of the inlet entrainer temperature increased acetone composition in distillate when the reflux ratio was higher than 4.0 (Figure 14). However, at temperatures higher than 50 °C the increase of the distillate composition was not significant. With respect to reflux ratio, it was observed that the highest distillate acetone composition was obtained at reflux rates of 4.0 and 5.0 (Figure 10), whereas at higher reflux rates acetone concentration in distillate decreases. This could be associated with the solvent feed stage. When it is fed near to the top of the column, it is mixed with the reflux, which causes the dilution of the entrainer and, therefore, the effectiveness decreases.

When the entrainer feed temperature was varied in the range of 20 to 100 °C, no effect on the distillate composition and condenser duty was observed (Figure 15). Nevertheless, the

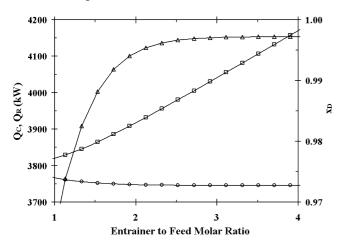


Figure 13. Entrainer to feed molar ratio effect on distillate composition (Δ) , and energy duty (condenser \bigcirc , and reboiler \square). Operating conditions: NS 52, BFS 48, EFT 47 °C, and R 5.0.

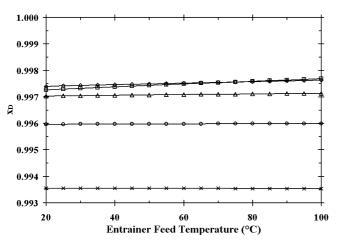


Figure 14. Entrainer feed temperature and reflux ratio influence on the distillate acetone mole composition. Operating conditions: NS 52, BFS 48, EFS 22, EFT 47 °C, and E/F 2.0. Evaluated refluxes: 3.0 (\times), 4.0 (o), 5.0 (Δ), 6.0 (\diamondsuit), y 7.0 (\square).

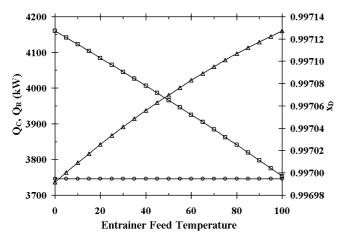


Figure 15. Entrainer feed temperature influence on distillate composition (Δ), and energy duty (condenser \bigcirc , and reboiler \square). Operating conditions: NS 52, BFS 48, EFS 22, EFT 47 °C, R 5.0, and E/F 2.0.

reboiler energy consumption was significantly affected by the inlet entrainer temperature. The reboiler duty decreased with the increase of the entrainer feed temperature because if entrainer is fed at low temperatures more energy is required to vaporize the liquid in the bottoms. When the solvent is fed at higher temperatures, small amounts of methanol are transferred to the

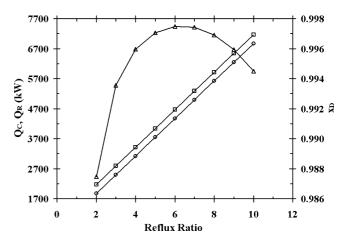


Figure 16. Reflux ratio effect on distillate composition (Δ), and energy duty (condenser \bigcirc , and reboiler \square). Operating conditions: NS 52, BFS 48, EFS 22, EFT 47 °C, and E/F 2.0.

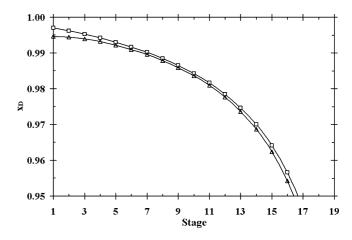


Figure 17. Pressure drop effect on acetone distillate composition (with a pressure drop of 0.01 atm, Δ; without pressure drop, □). Operating conditions: NS 52, BFS 48, EFS 22, EFT 47 °C, R 5.0, and E/F 2.0.

Table 2. Extractive Distillation Column Design

parameter	value
number of stages	52
binary feed stage	48
entrainer feed stage	22
reflux ratio	5
entrainer to feed molar ratio	2
entrainer temperature (°C)	47

Table 3. Methanol Recovery Column Design

parameter	value
number of stages	26
distillate mole flow (kmol/h)	25
feed stage	14
reflux ratio	3
bottoms temperature (°C)	104
distillate temperature (°C)	62

liquid phase and the liquid flow to the bottoms is lower. Figure 16 shows the effect of reflux ratio on distillate composition, and condenser and reboiler duties.

Finally, the pressure drop effect on acetone final composition is presented in Figure 17. The plot shows how the liquid profile composition in the extractive column was affected by a pressure drop neglected and $\Delta P = 0.01$ atm. The other operating conditions were established above. When $\Delta P = 0$ psi, distillate acetone composition was higher than the obtained when the column had a ΔP of 0.01 atm per stage. This is because when

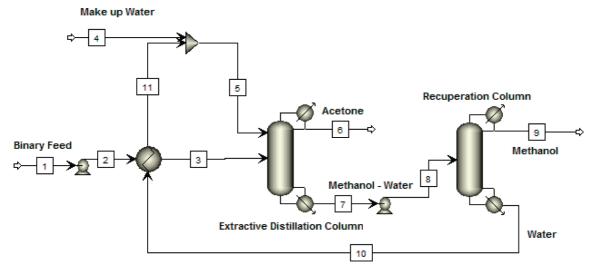


Figure 18. Process flow-sheet for extractive distillation of acetone-methanol using water as an entrainer.

Table 4. Feed Streams' Conditions

stream	1	4
feed mole flow (kmol/h)	100	1
temperature (°C)	20	47
pressure (atm)	1	1
mole fraction		
acetone	0.7775	0
methanol	0.2225	0
water	0	1

Table 5. Configuration of Extractive and Recovery Columns

parameter	extractive column	recovery column
number of stages	52	26
feed stage	48	14
entrainer feed stage	22	
reflux ratio	5	3
condenser	total	total
top stage pressure (atm)	1	1
pressure drop per stage (atm)	0.01	0.01
distillate mole flow (kmol·h ⁻¹)	76	25

Table 6. Simulation Results for the Process Flow-Sheet Presented in Figure $18\,$

			Mole Fraction		
	mole flow (kmol•h ⁻¹)	acetone	methanol	water	
1	20	100	0.778	0.223	0.000
2	20	100	0.778	0.223	0.000
3	64	100	0.778	0.223	0.000
4	47	1	0.000	0.000	1.000
5	47	200	0.000	0.000	1.000
6	56	76	0.995	0.003	0.003
7	94	224	0.010	0.098	0.892
8	94	224	0.010	0.098	0.892
9	62	25	0.086	0.882	0.032
10	104	199	0.000	0.000	1.000
11	47	199	0.000	0.000	1.000
				Extractive Column	Recovery Column
		N	Iole Fraction	n in Distillate	
			acetone	99.5%	8.6%
			methanol	0.3%	88.2%
			water	0.3%	3.2%
		N	Mole Fractio	n in Bottoms	
			acetone	1.0%	0.0%
			methanol	9.8%	0.0%
			water	89.2%	100.0%

a pressure drop is present in the column more energy is required to drive the vapor up through the distillation column, thus at

Table 7. Condenser and Reboiler Heat Duties on the Columns

	extractive column	recovery column
condenser (kW)	-3748	-975
reboiler (kW)	3858	987

the same conditions of energy supply the separation efficiency will be lower when a pressure drop is not neglected.

Configuration and operating conditions of the primary column was established from results obtained with the sensitivity

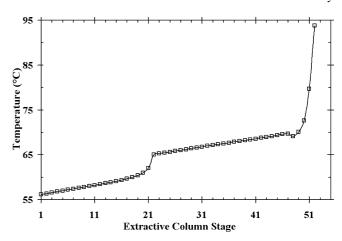


Figure 19. Extractive column temperature profile.

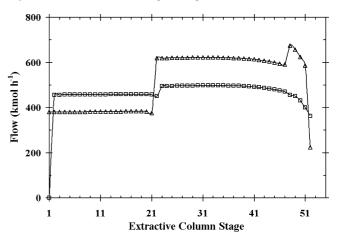


Figure 20. Liquid (Δ) and vapor (\Box) molar flow profiles in the extractive column.

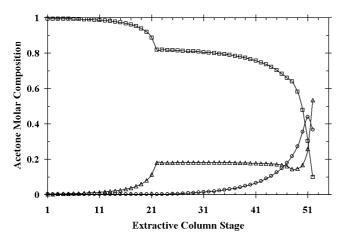


Figure 21. Vapor-phase concentration profiles of acetone (\Box) , methanol (\bigcirc) , and water (Δ) in the extractive column.

Table 8. Comparison of Simulation Results with Other Studies

parameter	Langston ¹¹	Luyben ⁸	Pradhan and Kannan ¹⁰	this study	
model	Wilson	UNIQUAC	UNIFAC	UNIQUAC	
acetone purity (%mol)	99.7%	99.4%	92.1%	99.0%	
E/F molar ratio	4	2	1.5	2	
	Extractive	Column			
number stages	73	57	20	52	
binary feed stage	5	40	10	48	
entrainer feed stage	25	25	3	22	
reflux ratio	4	3.44	4	5	
binary feed compos	sition (% mo	1)			
acetone	50	50	75	77.75	
methanol	50	50	25	22.25	
pressure drop per stage (atm)	0.02		0.01	0.01	
Recovery Column					
number stages	34	26		26	
feed stage	18	14		14	
reflux ratio	3.86	1.61		3	
pressure drop per stage (atm)	0.02			0.01	

analysis (Table 2). The best primary column configuration shows that the entrainer is fed above the binary feed, which allows us to obtain higher acetone purity. Similar results have been reported, 8,9 which suggests the use of this configuration for the separation of the minimum-boiling point azeotrope mixtures.

3.2. Simulation Results. Simulation of the acetone—methanol azeotropic mixture separation involves two columns: the extractive distillation column in which acetone of 99.5% mass (~99.0% mol) of purity is obtained and a recuperation column in which methanol is recovered. The recuperation column design

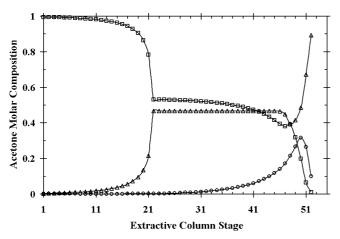


Figure 22. Liquid-phase concentration profiles of acetone (\Box) , methanol (\bigcirc) , and water (Δ) in the extractive column.

was initially done by means of short-cut column calculation (DSTWU) to establish the reflux ratio, number of stages, feed stage, and distillate mole flow (kmol h⁻¹), and results are presented in Table 3. Because of the high temperature of the bottom product (water), it is necessary to cool it before recycling at the beginning of the process. The proposed process flowsheet of the extractive distillation process is shown in Figure 18.

The simulation was carried out using a rigorous method (RadFrac). Tables 4 and 5 show the feed streams specifications and the extractive and recovery columns configuration, respectively.

The simulation results showed that the obtained acetone mole composition in the extractive column top was 0.99, whereas the acetone mole composition in the recuperation column was 0.099. The energy consumption on the extractive and recovery columns is presented in Table 7.

The temperature profile on the extractive column showed a temperature change at stage 22 due to the entrainer introduction, whereas at stage 48 the temperature had a minimal decrease because of the azeotropic mixture feeding. A significant temperature increase was observed at stages 51 and 50 due to the reboiler proximity (Figure 19). Figure 20 presents the vapor and liquid molar flow profiles in the extractive column. The liquid molar flow exposed two significant changes due to the entrainer and the azeotropic mixture feed at stages 22 and 48, respectively. Meanwhile, the vapor molar flow remained constant along the column, except at stage 22 in which the entrainer was fed. This change was caused by the liquid-phase vaporization due to the water inlet temperature.

In the vapor composition profile of the extractive column was observed that acetone concentration decreased at stage 22 in which the entrainer was fed. Methanol composition became appreciable at stage 23 and from this stage until the bottoms of the column the composition was increased. At stage 40, the observed change on methanol composition was due to the azeotropic mixture feed. The water profile had a significant change at stage 22 in which it is fed (Figure 21). The main product in the top of the column was acetone (light key component) and in the bottoms the principal compounds were methanol and water. Meanwhile, for the liquid molar compositions profiles, acetone and water had an important change at stage 22, in which the acetone composition decreased significantly and water increased due to the entrainer introduction. The azeotropic mixture feeding at stage 48 produced an increase in acetone composition, whereas a decrease in water composition was observed. The acetone composition was decreasing along the column and in the bottoms only water and methanol were present. Methanol exposed only one significant change at stage 48 in which the binary mixture was fed.

3.3. Comparison to Other Studies. The extractive distillation simulation for the system acetone—methanol—water has been reported. However, only in few reports the acetone purity obtained and the configuration of the columns is mentioned. Table 8 shows the comparison of simulation results with reported data.

The acetone purity obtained by Langston¹¹ is higher in comparison to obtain in the other studies. These differences could be due to the physical estimation property model. Langston¹¹ used the Wilson model for the simulation but in our previous work the experimental data showed that the most suitable model to predict the azeotrope of the binary mixture was UNIQUAC. Also, the design of both columns (extractive and recovery) is different and the total number of stages is higher for Langston. These differences could be due to assumptions

like pressure drop, different entrainer to feed molar ratio, binary mixture feeding composition, and reflux ratio.

Pradhan and Kannan¹⁰ obtained in the distillate stream the lowest acetone purity. This probably is caused by the reflux ratio (1.5) because this is not the optimum for acetone separation. Differences on reflux ratio and model used to estimate the system properties cause an extensive difference in the extractive column design. Pradhan and Kannan¹⁰ did not study the recovery column.

The preliminary design of the columns (extractive and recovery) for this work was taken from Luyben⁸ work, and physical property estimation model was the same. However, some important differences in the results between these works were observed, probably because the Luyben⁸ work did not take into account the pressure drop in the columns and additional adjustment to the operating conditions that were done as a result of the sensitivity analysis performed. Also, it can be observed that the feed composition is different in these two studies, suggesting the importance of correctly adjusting all of the different variables interacting and influencing the final design. The design obtained in the present work uses a more concentrated feed to the column, which is a realistic and typical case of the industrial plants, where mixtures are concentrated up to azeotropic composition and then they are submitted to the azeotropic separation processes to reduce energy consumption and size in this kind of separations.

The results of the simulations showed that the acetone purity in the distillate of the extractive column is affected by the boiling point difference between the light key component and the entrainer. In extractive distillation, the solvent must have a higher boiling point with respect to those of the azeotropic mixture components. Water has a boiling point greater than acetone and methanol but does not have a large volatility to guarantee the desired separation.

The ASTM standard specification for acetone is 99.5% mass and the purity obtained in this work was 99.51% mass, thus the purity restriction was achieved. However, to obtain best purity results another solvent could be studied.

4. Conclusions

This simulation work allowed us to determine the most suitable operating conditions for the separation of the azeotropic mixture acetone-methanol by extractive distillation using water as an entrainer. To obtain the best conditions and configuration for extractive and recovery columns, sensitivity analysis was done. The results of the simulation agree with those from literature. The temperature, composition, and molar flow profiles obtained for the extractive distillation column were consistent. Minimum energy requirements were obtained in compliance with the acetone purity restriction.

The separation of azeotropic mixtures like acetone—methanol is a feasible by extractive distillation if the solvent is selected properly. For this study, water was a feasible entrainer but the use of a solvent with a higher boiling point could be more appropriate for this azeotropic separation.

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