Computational study of the acetic acid extraction process from an aqueous solution with the aid of biological buffer

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Abstract. The liquid-liquid extraction of acetic acid from an aqueous solution with 1-heptanol as an extraction solvent in the extraction column and mixer-decanter at 30°C and atmospheric pressure was simulated using Aspen Plus. A Non-Random Two-Liquid (NRTL) based model was developed by minimizing maximum-likelihood objective function. In the simulation of the extraction column and mixer-decanter, the effect of the number of stages and the flow rate of the solvent on the percent recovery can be seen. In addition, a comparison of the percent recovery value between acetic acid extraction systems using EPPS (4-(2-hydroxyethyl)-1-piperazine propanesulfonic acid) and HEPES (4-(2-hydroxyethyl)-1 piperazineethanesulfonic acid) buffers was also carried out with systems without buffers. In this study, an economic analysis was also carried out for the acetic acid extraction system using an extraction column and a mixer-decanter. Based on the simulation results, the acetic acid extraction system with the addition of HEPES buffer using extraction column with the number of stages = 8 and solvent to feed mass ratio = 1.6 was the most optimal and efficient extraction process obtained in this study. This system has the capital cost of 180,729,262.67 USD with the percent recovery up to 99.83% and the mass fraction of acetic acid in the raffinate phase is 0.0002 which is also extremely low.

1. Introduction

Acetic acid, a second aliphatic compound, is an essential carboxylic acid used as a source of paints, plastics, adhesives, and food preservative. The majority consumption of acetic acid is used in the manufacture of polymers derived from polyvinyl acetate. Another important usage of acetic acid is to be used to make purified terephthalic acid for polyethylene terephthalic (PET) production [1]. The acetic acid market is expected to grow in the future as a result of the increased demand for polymers production. The demand for acetic acid was 16.3 m ton/year at the end of 2018. Marketwatch forecasts an annual growth rate of greater than 20% by 2024 in the global market [2].

Acetic acid is commonly produced via catalytic methanol carbonylation (CH₃OH + CO → CH₃COOH) and by bio-produced fermentation pathways [1]. Bio-produced fermentation pathway is the traditional method, which is used less by industries nowadays, typically because of separation and purification issues from fermentation broth is challenging. However, due to the fact that methanol is a
non-renewable material and the increasing demand of acetic acid reagents in the industry, the separation of acetic acid has attracted researchers to sustain acetic acid via bio-based production.

Various methods have been investigated to recover acetic acid from its aqueous solution including electro-membrane separation [1], vacuum membrane distillation [2], adsorptive membrane [3], electro-dialysis [4], and liquid-liquid extraction [5,6]. Major drawbacks of these technologies are high-production cost and concentration steps. Recently, Arias et al. [9] reported liquid-liquid extraction via salting-out induced extraction. The salting-out effect can lead to an increase in the distribution coefficient and selectivity [7]. Unfortunately, in the process of salting out, the high concentration of salts causes corrosion on the equipment [11]. It can also change the optimal pH of the extraction medium and cause denaturation of biomolecules. To overcome this problem, the addition of biological buffer can be applied on liquid-liquid extraction process to replace the use of salt, which is a non-corrosive and environmentally benign materials [12]. Besides, biological Good's Buffer can be used for separation process using liquid-liquid extraction in various type of aqueous solutions because it is biocompatible [9]. Good's buffer is a potential green agent that is useful for the recovery of organic solvents from their aqueous solutions with the help of a buffering-out effect [10]. EPPS is widely used as a zwitterionic buffer in biology and biochemistry research and its chemical structure contains a piperazine ring. It is useful for pH control as a standard buffer in the physiological region of 7.3 to 8.7 [9]. HEPES [4-(2-hydroxyethyl)-1 piperazineethanesulfonic acid] is a widely used biological buffer that becomes useful at pH range between 6.8 and 8.2 (pK~ = 7.5). In addition, the biological buffers keep the pH in the physiological region of pH 6 to 8. Therefore, the buffering-out phase separation could be a promising method for both the separation of biological materials such as proteins and the recovery of organic solvents from their aqueous solutions [9].

Hence, a process simulation is fundamentally important as an effective tool for understanding and developing acetic acid extraction process. The computational study of liquid-liquid extraction with selected biological buffer is employed to minimize loss of the valuable acetic acid. Several important parameters used in liquid-liquid extraction are distribution coefficient, solvent selectivity, and solvent or feed ratio [11]. In this study, the extraction column and mixer-decanter were simulated with a Non-Random Two-Liquid (NRTL) model using Aspen Plus V10 for liquid-liquid extraction of acetic acid from an aqueous solution using 1-heptanol as an extraction solvent at 30°C and atmospheric pressure. In the simulation of the extraction column and mixer-decanter, the effect of number of stages and solvent to feed ratio (flow rate of the solvent) on the percent recovery of acetic acid can be seen. In addition, a comparison of the percent recovery value between acetic acid extraction systems using EPPS (4-(2-hydroxyethyl)-1-piperazine propanesulfonic acid) and HEPES (4-(2-hydroxyethyl)-1 piperazineethanesulfonic acid) buffers was also carried out with systems without buffers. In this study, an economic analysis was also carried out for the acetic acid extraction system using an extraction column and a mixer-decanter.

2. Materials and method

2.1. Computational Study of Acetic Acid Extraction Process
Computational study of acetic acid extraction process from an aqueous solution was carried out on the extraction column and mixer-decanter equipment with the acetic acid content in the feed was fixed at 10% weight. ASPEN PLUS software (version 10) was used to simulate the liquid-liquid extraction of acetic acid from an aqueous solution using 1-heptanol as solvent at temperature of 30°C and atmospheric pressure (1 bar). The effectiveness of 1-heptanol as an extraction solvent was determined from the simulation parameters in terms of simulated counter-current liquid-liquid extraction and simulated mixer-decanter process. The NRTL thermodynamics model was chosen for the method of the simulation. Furthermore, the effects of the addition of EPPS and HEPES buffers on the percent recovery of acetic acid in the extract phase with the variation of number of stages and solvent to feed ratio were also studied. The concentration of biological buffer in the feed was also fixed at 15% weight. Figures 1 and 2 show a process flow diagram on the extraction column and mixer-decanter for acetic acid extraction using ASPEN PLUS V10.
2.2 Economic Analysis
The economic analysis was calculated based on the capital cost, including the equipment cost, the installed cost, and the material cost with the basis of annual production. The equipment and installation costs for extraction column were calculated using Guthrie’s cost correlations with Marshall and Swift index [12]. The Marshall & Swift index (M&S) is specified at 1518.1 (in year 2011) [13]. The economic analysis can be used for the evaluation in the application of extraction process in industry to determine the optimum process design by obtaining high percent recovery with the minimum capital cost.

3. Result and discussion
3.1 The Effect of The Number of Stages And Solvent to Feed Ratio on the Percent Recovery

3.1.1 Extraction Column
The effect of the number of stages and solvent to feed ratio (solvent flowrate) on the percent recovery in the extraction column for the acetic acid + water + 1-heptanol extraction system is shown in tables 1, table 2 and figures 3. Simulation of the extraction column was carried out using various amounts of stages from 3 to 8 and the mass ratio of solvent to feed was 1 (solvent flow rate = 25 kg/hr), 1.6 (solvent flow rate 40 kg/hr), and 2 (solvent flow rate 50 kg/hr). Based on table 1, the percent recovery of acetic acid increases from 50% to 56% along with the increase of the number of stages, with an increase of 1.03% at each stage. The binary parameters of NRTL model for the liquid-liquid equilibria of acetic acid + water + 1-heptanol system were determined in this study by regressing the experimental liquid-liquid equilibrium data of Darwish et al [14] by minimizing the maximum likelihood objective function as seen in table 3. The binary parameters obtained were applied in the simulation process for the extraction of acetic acid+water+1-heptanol systems using extraction column and mixer-decanter.
Table 1. Comparison of Percent Recovery for Acetic Acid + Water + 1-Heptanol System using Extraction column with solvent to feed mass ratio = 1

| Number of stages (N) | 3   | 4   | 5   | 6   | 7   | 8   |
|----------------------|-----|-----|-----|-----|-----|-----|
| Solvent to feed mass ratio | 1  | 1   | 1   | 1   | 1   | 1   |
| Acetic acid in raffinate (mass fraction) | 0.0579 | 0.0555 | 0.0541 | 0.0533 | 0.0527 | 0.0523 |
| Recovery of Acetic Acid in extract (%) | 50.71% | 52.95% | 54.22% | 55.02% | 55.53% | 55.88% |

While in table 2, the extraction column simulation was carried out using the variation of the number of stages from 3 to 8 and increasing the solvent flow rate to 40 kg/hr (solvent to feed mass ratio = 1.6). The increase in solvent to feed ratio causes an increase on percent recovery value. From the comparison in tables 1 and 2, all the percent recovery values of acetic acid increase due to the changes in solvent flow rate, in which the percent recovery ranges from 69% to 80% with an increase of 22.24% for each stage. Based on the percent recovery shown in table 1 and table 2, it can be concluded that increasing the mass ratio of the solvent to feed (solvent flow rate) can increase the percent recovery more significantly when compared to increasing the number of stages in the extraction column, because increasing the solvent flow rate can produce higher percent recovery. Although the value of the percent recovery of acetic acid in the extraction column increased due to the addition of the solvent flow rate, the simulation results were not efficient enough to be applied in the separation of acetic acid from the aqueous solution, because the percent recovery of acetic acid was still below 90%, which was still relatively low. Therefore, the mass ratio of solvent to feed must be increased to 2 (solvent flow rate = 50 kg/hour) to obtain a percent recovery of acetic acid up to 90.49% with the number of stages = 8, which can be seen in figure 3.

Table 2. Comparison of Percent Recovery for Acetic Acid + Water + 1-Heptanol System using Extraction column with solvent to feed mass ratio = 1.6

| Number of stages (N) | 3   | 4   | 5   | 6   | 7   | 8   |
|----------------------|-----|-----|-----|-----|-----|-----|
| Solvent to feed mass ratio | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| Acetic acid in raffinate (mass fraction) | 0.0392 | 0.0342 | 0.0309 | 0.0285 | 0.0268 | 0.0255 |
| Recovery of Acetic Acid in extract (%) | 69.57% | 73.62% | 76.30% | 78.17% | 79.54% | 80.57% |

Figure 3. Variation of percent recovery of acetic acid with the number of stages in the acetic acid + water + 1-heptanol system with solvent to feed mass ratio of 1, 1.6, and 2 using extraction column
Table 3. Optimal Values of the NRTL model parameters for the acetic acid (1) + water (2) + 1-heptanol (3) systems

| System | \( \alpha_{ij} \) | i-j | \( b_{ij}/K \) | \( b_{ij}/K \) |
|--------|------------------|-----|---------------|---------------|
| Acetic Acid (1) + Water (2) + 1-heptanol (3) | 0.2 | 1-2 | 1682.401 | 12.7208 |
|        | 0.2 | 1-3 | 507.0367 | 110000 |
|        | 0.2 | 2-3 | -13351.8 | 1050.06 |

3.1.2 Mixer and Decanter

The mixer and decanter can also be applied for the simulation of the liquid-liquid extraction of acetic acid from its aqueous solution using 1-heptanol solvent. As shown in table 4, table 5 and figure 4, the number of stages used in the Mixer and decanter simulation varied from 3 to 8 with a mass ratio of solvent to feed of 1 (solvent flow rate 25 kg/hour), 1.6 (solvent flow rate 25 kg/hour), solvent flow 40 kg/hour), and 2 (solvent flow rate 50 kg/hour). Based on table 4, using a mass ratio of solvent to feed of 1 (solvent flow rate 25 kg/hour) shows that the percent recovery of acetic acid increases from 62% to 71% along with the stage number increase with an increase of 1.80% at each stage.

Table 4. Comparison of Percent Recovery for Acetic Acid + Water + 1-Heptanol System using Mixer-Decanter with solvent to feed mass ratio = 1

| Number of stages (N) | 3  | 4  | 5  | 6  | 7  | 8  |
|----------------------|----|----|----|----|----|----|
| Solvent to feed mass ratio | 1 | 1 | 1 | 1 | 1 | 1 |
| Acetic acid in raffinate (mass fraction) | 0.0447 | 0.0408 | 0.0383 | 0.0366 | 0.0354 | 0.0346 |
| Recovery of Acetic Acid in extract (%) | 62.20% | 65.72% | 67.94% | 69.42% | 70.44% | 71.18% |

While in table 5, the simulation of the mixer-decanter column was carried out using a variation of the number of stages from 3 to 8 and increasing the solvent flow rate to 40 kg/hour (solvent to feed mass ratio = 1.6). Increasing the ratio of solvent to feed causes an increase in the value of percent recovery. From the comparison between table 4 and table 5, all values of the percent recovery of acetic acid increased due to changes in the solvent flow rate, where the percent recovery ranges from 80% to 93% with an increase of 20.76% for each stage. Based on the percent recovery shown in table 4, table 5 and figure 4, it can be concluded that it is better to increase the mass ratio of solvent to feed (solvent flow rate) to increase the percent recovery significantly when compared to increasing the number of stages in the extraction column due to an increase in flow rate. Solvent can produce a higher percent recovery value. Even if the solvent flow rate is increased to 50 kg/hour (mass ratio of solvent to feed = 2) it can produce a percent recovery of up to 98.11% at stage 8. With a percent recovery value of 98.11%, the separation of acetic acid from the aqueous solution can run optimally as shown in figure 4.

Table 5. Comparison of Percent Recovery for Acetic Acid + Water + 1-Heptanol System using Mixer-Decanter with solvent to feed mass ratio = 1.6

| Number of stages (N) | 3 | 4 | 5 | 6 | 7 | 8 |
|----------------------|---|---|---|---|---|---|
| Solvent to feed mass ratio | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| Acetic acid in raffinate (mass fraction) | 0.0252 | 0.0191 | 0.0150 | 0.0121 | 0.0099 | 0.0083 |
| Recovery of Acetic Acid in extract (%) | 80.43% | 85.29% | 88.61% | 90.82% | 92.50% | 93.79% |
3.2. The Effect of the addition of biological buffer on the recovery of acetic acid

3.2.1 Extraction Column Simulation

Based on table 1 and table 2, the percentage recovery value generated in the extraction column simulation is not high enough, which indicates that the simulation process is not efficient for the separation of acetic acid from its aqueous solution. Therefore, in this study, a biological buffer, namely EPPS or HEPES, was added to the acetic acid + water + 1-heptanol extraction system to increase the efficiency of the extraction process as indicated by the high percentage of acetic acid recovery in the extract phase. Table 6 shows the percent recovery in the acetic acid extraction system with the addition of EPPS and the variation of number of stages from 3 to 8 using a mass ratio of solvent to feed of 1.6 (solvent flow rate 40 kg/hour). Based on table 6, the percent recovery of acetic acid increased with a range of 94% to 99%, so it can be concluded that the simulation process of acetic acid separation using an extraction column with the addition of EPPS works more efficiently than the system without the addition of buffer, especially at stages 3 to 8 where the value the resulting percent recovery is above 90%.

Table 6. Comparison of Percent Recovery for Acetic Acid + Water + 1-Heptanol System with the addition of EPPS using Extraction column and solvent to feed mass ratio = 1.6

| Number of stages (N) | 3   | 4   | 5   | 6   | 7   | 8   |
|---------------------|-----|-----|-----|-----|-----|-----|
| Solvent to feed mass ratio | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| Acetic acid in raffinate (mass fraction) | 0.0074 | 0.0037 | 0.0019 | 0.0010 | 0.0006 | 0.0003 |
| Recovery of Acetic Acid in extract (%) | 94.25 | 97.13 | 98.52 | 99.21 | 99.57 | 99.77 |

In addition, HEPES is another buffer that can be used to optimize the extraction of acetic acid from aqueous solutions. Table 7 shows the percent recovery in the acetic acid extraction system with the addition of HEPES, the number of stages used is 3 to 8 and using a mass ratio of solvent to feed of 1.6 (solvent flow rate 40 kg/hour). Based on the results obtained, the percent recovery ranges from 94% to 99%, so it can be concluded that the simulation of the acetic acid extraction column with the addition of HEPES can also work efficiently, especially at stages 3 to 8 because it can produce a recovery percentage above 90%.

Figure 4. Variation of percent recovery of acetic acid with the number of stages in the acetic acid + water + 1-heptanol system with solvent to feed mass ratio of 1, 1.6, and 2 using mixer-decanter
Table 7. Comparison of Percent Recovery for Acetic acid + Water + 1-Heptanol System with the addition of HEPES using Extraction column and solvent to feed mass ratio = 1.6

| Number of stages (N) | 3   | 4   | 5   | 6   | 7   | 8   |
|----------------------|-----|-----|-----|-----|-----|-----|
| Solvent to feed mass ratio | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| Acetic acid in raffinate (mass fraction) | 0.0067 | 0.0032 | 0.0016 | 0.0008 | 0.0004 | 0.0002 |
| Recovery of Acetic Acid in extract (%) | 94.55 | 97.40 | 98.72 | 99.36 | 99.67 | 99.83 |

Figure 5. Variation of percent recovery of acetic acid with the number of stages in the acetic acid + water + 1-heptanol and acetic acid + water + 1-heptanol + biological buffer systems using extraction column (solvent to feed mass ratio = 1.6)

Based on figure 5, the percent recovery of acetic acid increased rapidly after the addition of EPPS with an increase of about 21.78% and after the addition of HEPES by 21.96% for each stage. From these results, it can be concluded that EPPS and HEPES have a positive effect on increasing the percent recovery. EPPS and HEPES are zwitterionic compounds that have very large dipole moment and can interact electrostatically with water. EPPS and HEPES have both hydrogen bond donor and acceptor sites. Therefore, EPPS and HEPES can strongly interact with water molecules through hydrogen bonding and electrostatic interactions [15]. Therefore, the interaction between acetic acid and water is reduced when the ions are dissolved. As the water molecules prefer to surround the ions from the buffer, they become unavailable for interaction with the acetic acid molecules, being a nonelectrolyte compound. As the result, the acetic acid molecules are buffering out from the aqueous solution and becomes more easily extracted into the organic solvent.

3.2.2 Mixer and Decanter
The addition of biological buffers, namely EPPS or HEPES, was also carried out on a mixer and decanter simulation in an acetic acid + water + 1-heptanol extraction system. Table 8 shows the percent recovery generated in the mixer and decanter simulation with the addition of EPPS buffer, while table 9 shows the percent recovery using a mixer and decanter with the addition of HEPES buffer. The number of stages used in the simulation of the mixer and decanter ranged from 3 to 8 with a mass ratio of solvent to feed 1.6 (solvent flow rate 40 kg/hour). Based on the results obtained, the percent recovery increased in the range of 86 to 97% for the acetic acid + water + 1-heptanol + EPPS
system and increases in the range of 94 to 99% for the acetic acid + water + 1-heptanol + HEPES system. Although the percent recovery has not reached 90% in stage 3 for the system with the addition of EPPS, the percent recovery generated in the mixer and decanter simulation with the addition of the EPPS buffer is much higher than the system without buffer as shown in table 4.

**Table 8.** Comparison of Percent Recovery for Acetic Acid + Water + 1-Heptanol System with the addition of EPPS using Mixer-Decanter and solvent to feed mass ratio = 1.6

| Number of stages, N | 3   | 4   | 5   | 6   | 7   | 8   |
|---------------------|-----|-----|-----|-----|-----|-----|
| Solvent to feed mass ratio, ns/nf | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| Acetic acid in raffinate | 0.0189 | 0.0128 | 0.0089 | 0.0065 | 0.0048 | 0.0036 |
| Recovery of Acetic Acid in extract (%) | 86.38 | 90.96 | 93.72 | 95.50 | 96.69 | 97.52 |

**Table 9.** Comparison of Percent Recovery for Acetic Acid + Water + 1-Heptanol System with the addition of HEPES using Mixer-Decanter and solvent to feed mass ratio = 1.6

| Number of stages (N) | 3   | 4   | 5   | 6   | 7   | 8   |
|----------------------|-----|-----|-----|-----|-----|-----|
| Solvent to feed mass ratio | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 | 1.6 |
| Acetic acid in raffinate (mass fraction) | 0.0066 | 0.0031 | 0.0015 | 0.0007 | 0.0004 | 0.0002 |
| Recovery of Acetic Acid in extract (%) | 94.61 | 97.47 | 98.78 | 99.40 | 99.70 | 99.85 |

**Figure 6.** Variation of percent recovery of acetic acid with the number of stages in the acetic acid + water + 1-heptanol and acetic acid + water + 1-heptanol + biological buffer systems using mixer-decanter (solvent to feed mass ratio = 1.6)

Based on figure 6, the percent recovery of acetic acid increased with the addition of EPPS about 4.89% for each stage. Meanwhile, the extraction system with the addition of HEPES also experienced an increase in the percent recovery of around 9.73% for each stage. From these results, it can be concluded that the mixer and decanter simulation for acetic acid extraction with the addition of HEPES can work efficiently, especially at stages 3 to 8 with the recovery of acetic acid percentage above 90%.
3.3. Economic Analysis
Based on the value of percent recovery in the acetic acid extraction system in both the extraction column and the mixer-decanner simulation, there are several systems that produce acetic acid recovery above 95%. Therefore, it is necessary to conduct an economic analysis that can be used for evaluation in the application of the extraction process in industry to determine the optimum process design by obtaining a high percent recovery with minimum capital costs. Based on the results of the economic analysis listed in Table 10, it can be concluded that the most optimal and efficient process is the acetic acid extraction system with the addition of HEPES buffer using an extraction column with a number of stages = 8 and a mass ratio of solvent to feed = 1.6 (solvent flow rate 40 kg/hour). This system has a capital cost of 180,729,262.67 USD with a percent recovery of up to 99.83% and the mass fraction of acetic acid in the raffinate phase is 0.0002 which is also extremely low.

Table 10. Variation of capital cost for extraction system with percent recovery >95%

| System                  | Number of Stages | Solvent to feed mass ratio (solvent flow rate) | Recovery of Acetic Acid in extract (%) | Acetic Acid in raffinate (%) | Capital cost (USD) |
|-------------------------|------------------|-----------------------------------------------|---------------------------------------|-----------------------------|-------------------|
| Acetic Acid + water + 1-heptanol + EPPS (extraction column) | 4                | 1.6 (40 kg/hr)                                | 97.13                                 | 0.0037                      | $ 201,482,211.40  |
|                         | 5                |                                               | 98.52                                 | 0.0019                      | $ 201,483,228.35  |
|                         | 6                |                                               | 99.21                                 | 0.0010                      | $ 201,489,788.26  |
|                         | 7                |                                               | 99.57                                 | 0.0006                      | $ 201,491,088.87  |
|                         | 8                |                                               | 99.77                                 | 0.0003                      | $ 201,499,376.56  |
| Acetic Acid + water + 1-heptanol + HEPES (extraction column) | 4                | 1.6 (40 kg/hr)                                | 97.40                                 | 0.0032                      | $ 180,712,097.51  |
|                         | 5                |                                               | 98.72                                 | 0.0016                      | $ 180,713,114.45  |
|                         | 6                |                                               | 99.36                                 | 0.0008                      | $ 180,719,674.37  |
|                         | 7                |                                               | 99.67                                 | 0.0004                      | $ 180,720,974.98  |
|                         | 8                |                                               | 99.83                                 | 0.0002                      | $ 180,729,262.67  |
| Acetic Acid + water + 1-heptanol (mixer-decanner) | 6                | 2 (50 kg/hr)                                  | 96.06                                 | 0.0054                      | $ 148,587,357.58  |
|                         | 7                |                                               | 97.23                                 | 0.0038                      | $ 148,613,654.48  |
|                         | 8                |                                               | 98.11                                 | 0.0027                      | $ 148,639,951.38  |
| Acetic Acid + water + 1-heptanol + HEPES (mixer-decanner) | 4                | 1.6 (40 kg/hr)                                | 97.47                                 | 0.0031                      | $ 180,807,846.26  |
|                         | 5                |                                               | 98.78                                 | 0.0015                      | $ 180,834,143.16  |
|                         | 6                |                                               | 99.40                                 | 0.0007                      | $ 180,860,440.06  |
|                         | 7                |                                               | 99.70                                 | 0.0004                      | $ 180,886,736.96  |
|                         | 8                |                                               | 99.85                                 | 0.0002                      | $ 180,913,033.86  |
| Acetic Acid + water + 1-heptanol + EPPS (mixer-decanner) | 6                | 1.6 (40 kg/hr)                                | 95.50                                 | 0.0065                      | $ 201,630,553.96  |
|                         | 7                |                                               | 96.69                                 | 0.0048                      | $ 201,656,850.86  |
|                         | 8                |                                               | 97.52                                 | 0.0036                      | $ 201,683,147.76  |

4. Conclusion
In this study, it can be concluded that the number of stages and solvent to feed ratio (solvent flow rate) used in the extraction column and mixer-decanner simulations has an influence on the percent...
recovery. According to the results obtained in this study, the values of percent recovery generated in the simulations for the systems without the addition of buffer are not high enough showing that the simulation process is not efficient for the separation of acetic acid from its aqueous solution. Therefore, it is necessary to add EPPS or HEPES buffer to increase the percent recovery. For the various extraction systems that were simulated on Aspen Plus V10, the most optimal and efficient process was the acetic acid extraction system with the addition of HEPES buffer using extraction column with the number of stages = 8 and solvent to feed mass ratio = 1.6. This system has the capital cost of 180,729,262.67 USD with the percent recovery up to 99.83% and the mass fraction of acetic acid in the raffinate phase is 0.0002 which is also extremely low.

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