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Modeling and simulation of ethanol extractive distillation process of COCAFE plant using Aspen HYSYS

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ABSTRACT

Extractive distillation is used an alternative method for anhydrous ethanol production, which has been observed to be more productive than that of existing process of COCAFE plant and, almost, to be very viable and feasible against the process that uses adsorption with molecular sieves and azeotropic process. Cyclohexane has turned out efficient solvent in extractive distillation. In this research, an extractive distillation process with solvent recovery unit was modelled and simulated with the Aspen HYSYS platform, to analyses the effect of different operating parameters such as flow rate, temperature, and pressure on production of the ethanol-water mixture composition and economic. In this work, the Peng Robinson fluid package was used to calculate different thermodynamic properties for the above-mentioned mixture. A comprehensive simulation model of the extractive distillation process was developed, along with a recovery column and a recycle loop. Different parameters such as feed flow rate, feed temperature and feed pressure changed with respect to mole percent of downstream ethanol production. The most satisfactory composition for the hydrous ethanol mixture was 0.996 mole percent of ethanol and 0.01 mole percent of water at 203 m^3/h feed flow rate. Finally, economic evaluation and energetically efficient operating conditions of entire model were carried out via in-built features of Aspen HYSYS.

Keywords:

Process simulation
Extractive distillation
Economic evaluation

1. Introduction

Anhydrous ethanol is widely used in the chemical industry as a raw material in chemical production of esters and ethers, and as solvent in production of paint, sprays, perfumery, medicine cosmetics, , and food, among others. Furthermore, mixtures of anhydrous ethanol and gasoline may be used as fuels, reducing environmental contamination, and improving gasoline's octane number, mainly due to the addition of ethanol [1].

Extractive distillation using cyclic solvents as entrainers is one of the most commonly used separation techniques for azeotropic mixtures in the chemical industry. To reduce the large energy

requirements, and the secondary pollution problems, extractive distillation using cyclohexane as solvent has become valuable process in ethanol dehydration [2].

Besides, Process simulation tools have become a very useful way in the design, analysis and retrofit of processes of interest from energy efficient to economical point of view, opening the possibility to make different sensitivity analyses and to combine optimization studies, cost estimation, detailed design, and controllability analysis [3].

Biofuels industry and the bioethanol production process are gaining ground owing to fast and easy, accuracy and reliability of modern technologies. In this regard, ethanol is one of the much-sought biofuels due to minimum environmental effects as compared to fossil fuels. Moreover, their environment-friendly properties and its renewable characteristics ensure environmental sustainability. In the final dehydration steps the purity of ethanol is determined by varying the operating conditions, the technology used, and its benefits related to the quality and costs of ethanol. In Brazil and United States, the two largest producers of ethanol in the world, azeotropic distillation, and extractive distillation with cyclohexane and adsorption with molecular sieves are used in dehydration of ethanol [4].

Apart from this, dehydration of ethanol offers challenge to the engineers, industrialists, experts, researchers, and innovators. Anhydrous ethanol is premium for ethanol blend in gasoline and other desired products. For blending with gasoline, ethanol must have at least 99.2% purity. Thus, to enhance its purity, ethanol is dehydrated after distillation via several contemporary process such as extractive distillation or pervaporation, azeotropic distillation and membrane technology. Considerable work on dehydration of ethanol has been done to date; however, the modeling and simulation of ethanol dehydration of most adopted process around the globe is very scant and countable. In short, this is the void which is intended to be filled through this research work. Therefore, this research will mainly focus on modeling and simulation of dehydration process and their comparative study.

The process simulators as Aspen HYSYS has its origin in the petrochemical industry and their use in other sectors depends on the validation of thermodynamic packages and the adaptation or development of new simulation blocks [5].

Process simulator Aspen HYSYS has been used in technical and economic analysis of several processes. Those include biodiesel production from vegetable oils, control setting evaluation of a depropanizing process, the study of extractive distillation processes of the mixture isobutyl

isobutanol-acetate at an industrial plant, simulation of sugarcane juice evaporation system for bioethanol production, conceptual processes involving acetone-methanol methyl-methanol acetate, and methanol-chloroform binary systems [6].

In an industrial distillation process, hydrous ethanol from fermentation unit goes through a distillation process in order to obtain hydrous ethanol with 99.02 ± 0.6. The ethanol consists of a complex mixture mainly including ethanol and water which forms the azeotrope. In this context, a simplified model of extractive distillation system was developed and solved with Aspen HYSYS. The findings exhibit the effective model for COCAFE plant, compared to already-established azeotropic model. This was the suggestion proposed to reflect the manner that distillation columns are heated in industrial plants. The results obtained with the model were compared with data from an industrial plant in order to evaluate if the approach presented in this work could be used to represent the real bioethanol distillation process.

2. Methodology

The required data was collected from COCAFE plant during the early phase of the research. These data are documented and used as the inputs for the simulation run of the project using Aspen HYSYS software. Initially, simulation run was done based on the typical model of ethanol dehydration unit. Property package used in running the simulation is carefully determined in order to increase the efficiency of the process, especially purity of ethanol on overhead products. The operating data of COCAFE plant for ethanol dehydration process were involved in the process in order to determined simulation results. These data are adjusted accordingly until the process simulation is fully converged. For the thermodynamic properties and equations, the under-mentioned fluid package was brought into consideration. The Peng-Robinson equation of state was used, as it is the recommended thermodynamic property package for hydrocarbon systems.

$$P = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}(\hat{v} + b) + b(\hat{v} - b)} \qquad (01)$$

Whereas, P= Pressure, T=Temperature, R=General Gas Constant and v'=specific volume.

The modeled, converged and simulated extractive process of COCAFE plant is shown in Fig. 01.

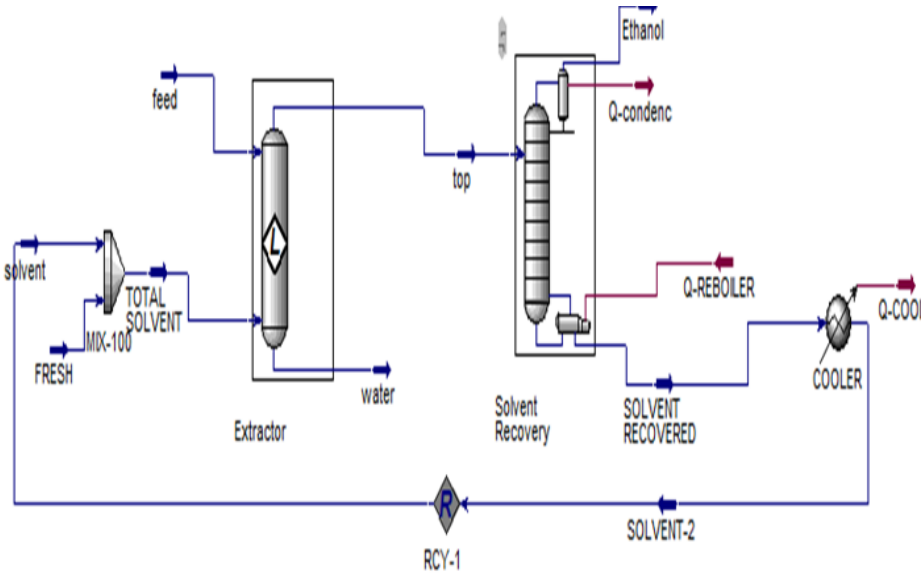

Fig. 01: The converged process of extractive distillation

The complete extractive and azeotropic distillation processes for anhydrous ethanol production were modeled and simulated using the Aspen HYSYS simulator V11 at a steady state. Extractive distillation is fed with a mixture of ethanol and water at different operating parameters, where a minimum-boiling homogeneous azeotrope is formed at 78.16 °C [1]. The Peng-Robinson was the physical property model chosen to describe the nonideality of both processes. In azeotropic distillation, a new azeotrope (ternary and heterogeneous) must be formed, generating in most cases two liquid phases and one vapor phase in the upper plates of the column.

In the extractive distillation, cyclohexane solvent, having high hydrophilic affinity, is continuously added at the top to separate the FEED at 91.29 ^{o}C, composed of ethanol and water, in the 1st column, producing high-grade ethanol (ETHANOL) in the top of the 1st column. The BOTTOM of the 1st column is mainly composed of the solvent and little amount of water, which enters the 2nd column to recover the WATER at the top and to recycle the solvent into the 1st column to keep the process continuous. This solvent can alter the relative volatility of the components, having a higher affinity to one of them, thus extracting it [1]. In this case, cyclohexane has a greater affinity with water.

The heater was kept at 80 °C to avoid spending much more energy with the junction of the streams. The MAKEUP stream closes the molar balance. Azeotropic distillation also works with a mixture of ethanol and water at atmospheric pressure, having the same minimum-boiling homogeneous

azeotrope at 78.16 °C, but the heterogeneity comes from the ternary azeotrope formed between ethanol, water, and the solvent (cyclohexane).

The cyclohexane was chosen as the entrainer due to its less toxicity when compared to benzene and ethylene glycol, the former entrainer used in this type of simulation [7].

In table 01, the feed composition of COCAFE plant is enlisted which was used in this research work determining the efficiency of extractive process, comparing the azeotropic model for the same conditions.

Table 01: Feed Composition

COMPONENT	**COMPOSITION (MOLE PERCENT)**
Ethanol	0.40
Water	0.40
Cyclohexane (solvent)	0.20

Again, table 02 shows the operating parameter for which both extractive and azeotropic processes for COCAFE plant were simulated. The table is given below.

Table 02: operating parameters of COCAFE plant

PARAMETER	**VALUE**
Flow Rate m^3/hr	203
Temperature (ºC)	91.29
Pressure (kPa)	98.09

In Table 02, the value of the flow rate is to initiate the simulation, and its balance is made through a convergence block in the ASPEN HYSYS. After defining the streams of the process, the characteristics of the extractive and azeotropic distillation columns are established. The number of stages, feed stage, and solvent stage of the extractive distillation columns were set by default for the sake of optimization. The distillate flow rate and reflux ratio for this

process was also optimized in the simulator. In the case of the azeotropic distillation columns, the high purity defined by the user causes the range of column operating conditions to be limited, not

being possible to optimize through sensitivity analysis. The optimization of the reflux ratios, feed stages, and solvent stages were manually made in the simulator to reach the high purity desired. Then, only the bottom flow rates were possible to be optimized in the simulator through design specs. Also, it is essential to mention that most works of extractive and azeotropic distillation processes in the literature use the range of 20 to 50 stages. [1] Then, it was considered for the optimization of the azeotropic distillation by the user, since the extractive distillation has the number of stages optimized by sensitivity analysis.

For the evaluation of steady state results using the simulation environment for the complete process of extractive distillation, comparisons were made with simulation results obtained from azeotropic process- the installed process of COCAFE industry [8]. For the evaluation of the steady state results produced by the simulation for extractive and conventional distillation, comparisons were made with industrial data to validate the models. Both simulators used Peng-Robinson for the calculation of activity coefficient and other thermodynamic properties for the said processes.

3. Results and discussion

The simulation models were made for complete extractive and azeotropic distillation processes, taking into account both a solvent recycle stream and a makeup stream to replenish whatever small amount of solvent may have been lost in the distillate product of the conventional column. This makeup stream was a necessity in order to obtain convergence. Specifications for an instance of this process can be found in Table 01 (where stage 1 is the top of the column, condenser and reboiler are considered stages, and “Bottoms product of extractive column” are values obtained from the bottoms product stream of the extractive column), where desired values specified by the user in the simulators were 309.6 kmol/h in the extractive column (the total amount of ethanol fed, desired as the distillate product) and 240 kmol/h in the conventional column (the total amount of cyclohexane fed into the extractive column), and the reflux ratio of both columns. The results for this simulation can be seen in figs. 02 and 03, for the extractive and conventional columns, respectively, demonstrating the effect of both the flowrate and temperature.

3.1. Effect of feed flow rate on ethanol production

In both azeotropic and Extractive model, 203 m^3/hr is the optimum point. However, after this flow rate, the ethanol mole percent drops due to solvent saturation and temperature sensitivity in extractive and azeotropic model respectively.

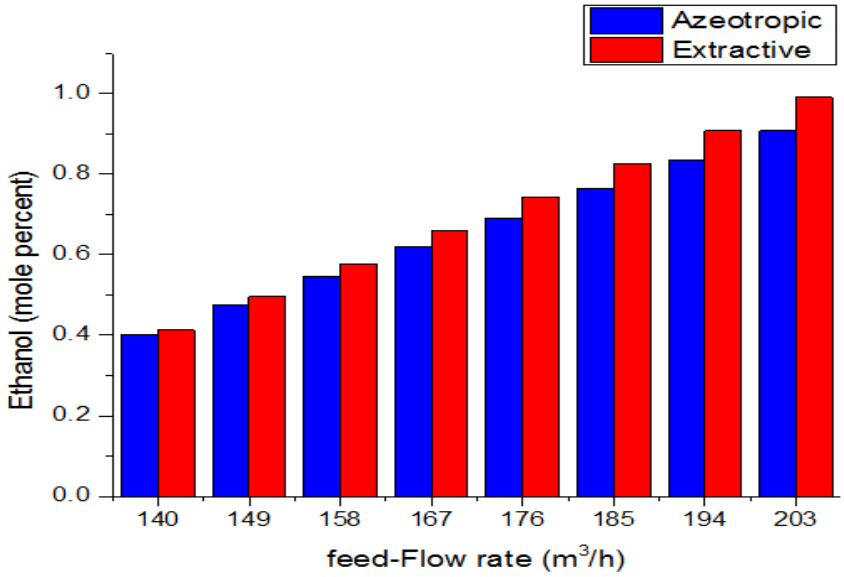

Fig. 02: Ethanol (mole percent) vs feed flowrate (m^3/h

It was observed from the results that COCAFE plant at present produces 0.9078 mole percent, compared with 0.9906 mole percent in Extractive process at 203 m^3/hr.

3.2. Effect of feed temperature on ethanol production

Similarly, as soon as the temperature reaches 100 $^{\circ}$C, the water evaporates with ethanol and the amount in WATER stream starts diminishing which results in lesser purity of ethanol in the end. Simulation results demonstrate that extractive distillation produces 0.406 mole percent of ethanol at 91 $^{\circ}$C whereas, Zeotropic germinates 0.398 mole percent for the same temperature. Thus, extractive bids fair prospect than that of azeotropic model.

3.3. Effect of feed flow rate w.r.t water in the bottom stream

In the same way, water percent in overhead product decreases as soon the flow rate increase till 203 m^3/hr flow rate. Right after the cited flow rate, the water content in Bottom Stream starts decreasing but the same increase in overhead products. However, the efficiency rests with extractive model.

3.4. Effect of feed-temperature on water content in bottom stream of distillation column

Moreover, Feed temperature has great impact on both models *i.e.*, azeotropic and extractive model. At 91 ^{O}C feed temperature, the extractive process generates 0.719 mole percent of ethanol followed by azeotropic with 0.689 mole percent.

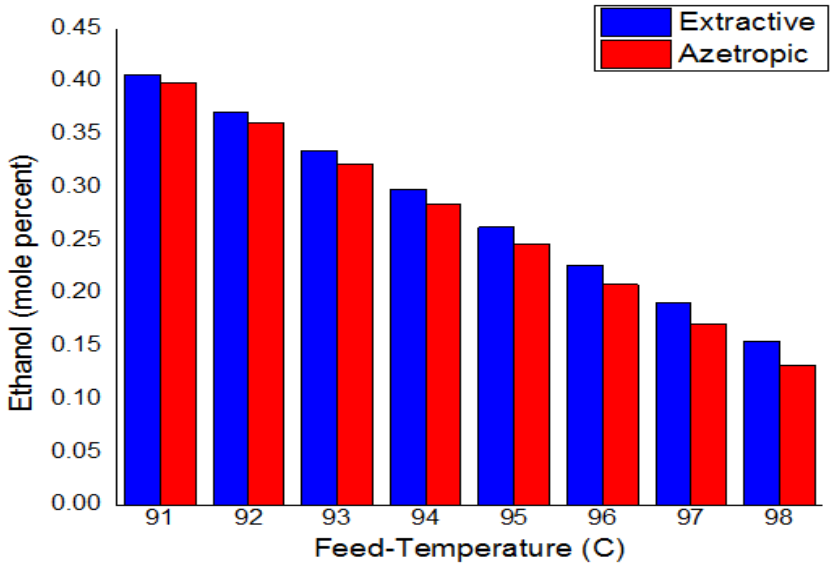

Fig. 03: Ethanol (mole percent) vs Temperature (ºC)

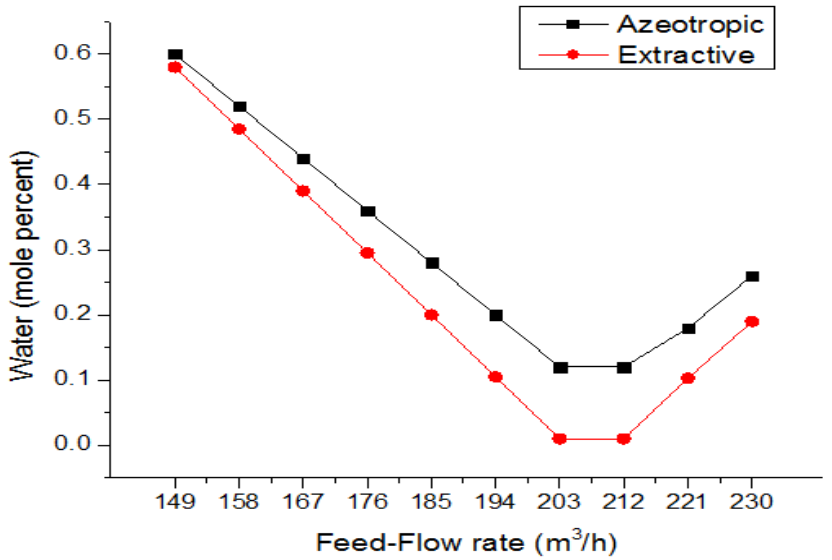

Fig. 04: Water in Bottom Stream (mole percent) vs feed flowrate (m^3/h)

Therefore, Water in the bottom stream reduces as temperature increases because water evaporates and is being carried away along with ethanol in overhead product, results in inefficiency of the processes.

3.5. Feed temperature effect on power consumption

Lastly, the condensers and reboilers receive already-hot substance. For which their duty reduces. The findings of simulation results show that the greater the feed temperature, the lesser will be the

cumulative energy consumption. At 91 ºC, the extractive model consumes 56.42 Kw , compared to 56.92 kw in azeotropic model. Thus extractive model is more efficient than that of azeotropic in COFAE plant.

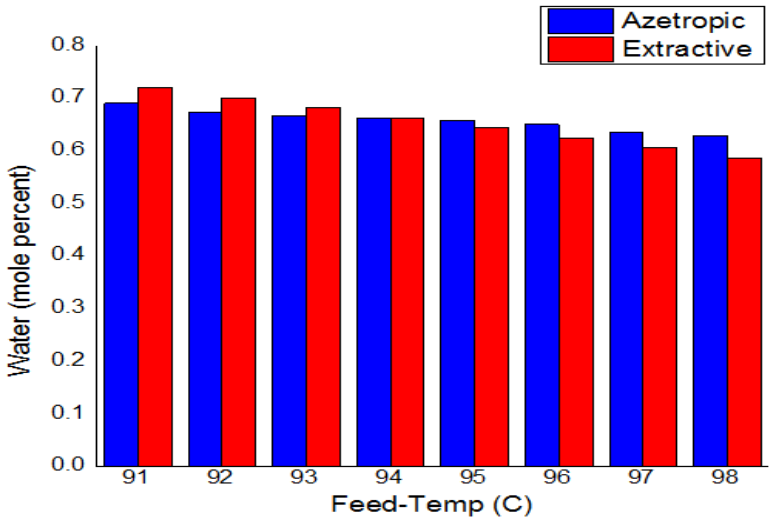

Fig. 05: Water in Bottom Stream (mole percent) vs Temperature (ºC)

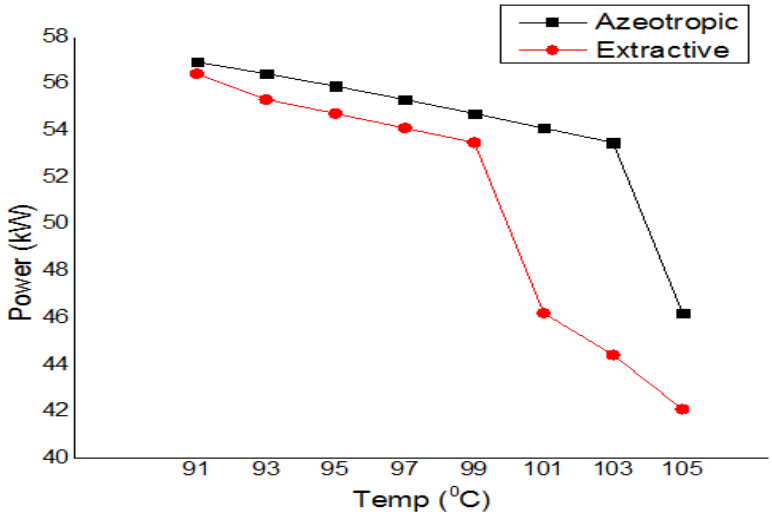

Fig. 06: Power consumption (kW) vs feed temperature (°C)

4. Conclusion

This work assessed the use of extractive and azeotropic distillation processes to produce anhydrous ethanol. Both processes demonstrated to be efficient regarding the purity of the anhydrous ethanol, achieving purities of 99.49 and 99.99 % of ethanol in the extractive and azeotropic distillations,

respectively. Nevertheless, when comparing both processes, the extractive is more advantageous than the azeotropic distillation concerning the reboiler heat duty, which the latter was 2.4 times higher. Both processes achieved the purities required for the anhydrous ethanol by the standard norms. The results were compared to the theoretical data in the open literature. One of the important contributions of this work was to build up the simulation involving recycles, and convergence strategy.

Comparative study of both models indicate that Extractive process is more efficient than that of already-embedded azeotropic model in COCAFE plant. In short, extractive model enjoys ascendency in ethanol dehydration concerning the COCAFE plant.

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