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SIMULATION OF ANHYDROUS BIOETHANOL PRODUCTION PROCESS USING EFFICIENCY CORRELATIONS FOR CONVENTIONAL AND EXTRACTIVE DISTILLATION

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Abstract
In this work, simulations of the complete separation process in anhydrous bioethanol production were carried out in Aspen Plus®. This process comprises distillation and rectification columns as well as an extractive column. Equilibrium stage model and Barros & Wolf efficiency correlations were used to perform the calculations. Efficiency profiles were obtained for all columns showing that efficiency values significantly vary along the columns. Influence of the introduction of efficiencies was evaluated through comparison with equilibrium stage model (ideal process). Results pointed out that energy requirements are not significantly higher when efficiencies are taken into account; however stream results and temperature profiles were quite different from each other. This reveals that is necessary to consider efficiency changes along the column if reliable predictions are to be made.

Keywords: Distillation, extractive distillation, efficiency, bioethanol

1. Introduction

Bioethanol plays an important role in the sustainable development, since it is a renewable fuel and originates less pollutant gases when compared to fossil-derived fuels. In this context, bioethanol can be used as substitute or in a mixture with gasoline. In Brazil, it is typically produced through fermentation of sugars derived from sugarcane and the separation step to obtain anhydrous bioethanol has a significant impact on the product cost.

In Brazilian biorefineries, wine obtained from fermentation stage is concentrated by means of a set of distillation and rectification columns, on which hydrous bioethanol (93 wt%) is obtained. Subsequently, due to the azeotrope formed by ethanol and water (95.6 wt% ethanol at 1 atm), dehydration processes are required to obtain anhydrous bioethanol (99.5 wt%) and the most usual process, nowadays in large scale industrial units, is the azeotropic distillation with cyclohexane, followed by extractive distillation with ethyleneglycol (EG). Compared to azeotropic distillation, extractive distillation requires less energy and is easier to operate, since it does not present two liquid phases inside the column.

Due to the fact that distillation operations demand a significant amount of energy and have a great importance in bioethanol production, the simulation of this unit operation has to be as representative as possible. In fact, reliable simulations allow the study of the distillation columns behavior and the optimization of the process, so the results can be put into practice in real facilities.

Usually, simulations of distillation process consider the equilibrium stage model, although, in practice, columns rarely operate under thermodynamic equilibrium conditions. In this context, rate-based model (or nonequilibrium stage model) provides the most accurate predictions; however, this rigorous model is more complex and involves a larger number of equations, thus increasing computational time, which is not desirable in online control applications. For this reason, consideration of efficiencies can be quite useful, provided that they are estimated properly. Among the available correlations, the Barros & Wolf efficiency correlations – obtained through adjustment of the mixture properties, such as thermal conductivity, density, heat capacity and diffusivity – can be used to calculate efficiencies for conventional and extractive distillations[1,2].

In this work, simulations of the separation process for bioethanol production were carried out in Aspen Plus® considering equilibrium stage model and the application of efficiencies determined by Barros & Wolf correlations. This work analyzes the influence of incorporating efficiency in column calculations.

2. Process Description

1.1 Hydrous Bioethanol Production

In order to produce hydrous bioethanol, most Brazilian biorefineries employ the configuration depicted in Figure 1, which consists of a series of distillation and rectification columns. Initially, the wine produced in the fermentation stage is fed to column A1 originating the top and bottom products that are sent to column D and A, respectively. Column D is responsible for removing volatile contaminants at the top, whereas column A removes large amounts of water (stillage or vinasse) in the bottom. Vapor phlegm produced near to the top of column A and liquid phlegm obtained at the bottom of column D are sent to rectification columns (column B-B1). The task of the rectification section is to concentrate the phlegm streams from 40-50 wt% to 93 wt% ethanol (hydrous bioethanol, “HE”). Sidestreams are withdrawn from column B-B1 and correspond to fusel oil, which is mainly characterized by isoamyl alcohol presence.

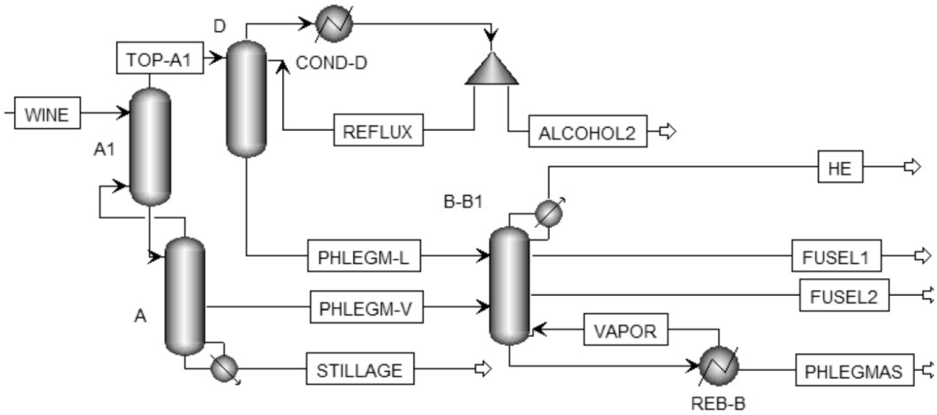

Figure 1. Configuration of the conventional distillation process

1.2 Anhydrous Bioethanol Production

In this work, the extractive distillation process with ethyleneglycol (EG) as solvent was considered as the method to separate the azeotropic mixture in order to produce anhydrous bioethanol. Extractive distillation, also known as homogeneous azeotropic distillation, is commonly used to separate nonideal mixtures with close boiling point or azeotropes. In this process, a heavy boiling solvent is added to the system to be separated, which alters the volatility of the component in the original mixture. Care has to be taken in the choice of the solvent since new azeotropes must not be formed and the solvent must be completely miscible in the mixture; in other words, it must not form a second liquid phase as in heterogeneous azeotropic distillation[1,3]. The conventional configuration employed in bioethanol production process is shown in Figure 2.

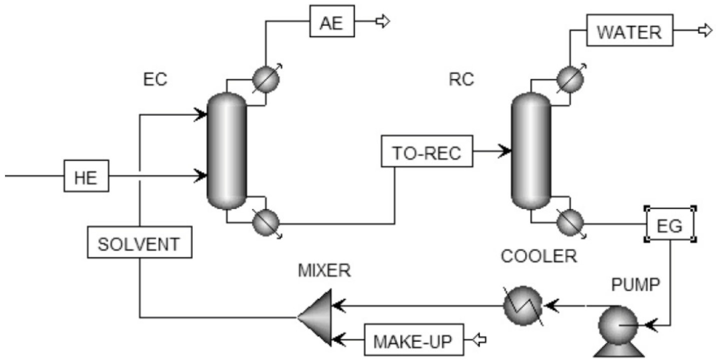

Figure 2. Configuration of extractive distillation process

As can be seen in Figure 2, solvent is fed to the first column (extractive column, “EC”), above the azeotropic feed. Anhydrous ethanol is produced on the top of the extractive column, while in the bottom a mixture containing solvent and water is obtained. The solvent is recovered in a second column (recovery column, “RC”), which is operated under vacuum (0.5 bar), then cooled and recycled to the first column.

3. Efficiency Correlations

Several works have shown the deviations of the equilibrium stage model results from experimental data[4,5,6]. In order to correct this weakness, efficiency can be introduced in the equilibrium calculations. For instance, efficiency correlations were developed by Barros[7] based on techniques of factorial design. These correlations, known as Barros & Wolf efficiency correlations, were proposed for conventional (Equation 1) and extractive (Equation 2) distillation processes.

$$\mathrm{Eff}(i) = 38.5309\left[\frac{k(i)\rho(i)D(i)MW(i)}{Cp(i)\mu^2(i)}\right]^{-0.04516} \tag{1}$$

$$\mathrm{Eff}(i) = 19.37272\left[\frac{k(i)\rho(i)D(i)MW(i)}{Cp(i)\mu^2(i)}\right]^{-0.109588} \tag{2}$$

In Equations 1 and 2, Eff (i) is the plate efficiency, which is a function of the following properties of the mixture: thermal conductivity (k), density (ρ), diffusivity (D), molecular weight (MW), heat capacity (Cp) and viscosity (μ).

Wolf-Maciel and collaborators[2] evaluated the performance of the Barros & Wolf efficiency correlation for a conventional distillation column using ethanol-water system. Comparison with nonequilibrium stage model and experimental data were carried out and a satisfactory agreement was achieved, validating the use of Barros & Wolf efficiency correlation. Similarly, Reis and coauthors[1] validated Barros & Wolf efficiency correlation for extractive distillation columns.

4. Simulation procedure

For calculations, NRTL model was used for the estimation of activity coefficients and vapor phase was considered ideal, since previous work about thermodynamic characterization has showed the adequacy of this model.

Typical industrial compositions of wine and hydrous bioethanol were considered the same for both approaches and are shown in Table 1. Additionally, configurations of the conventional and extractive distillation processes used in the simulations are those depicted in Figures 1 and 2, respectively. Column specifications are given in Table 2 and 3. Stages numbering initiates from the top stage or condenser, when it is present and coupled reboiler is considered the last stage.

Correlation for conventional columns (Equation 1) was used to determine plate efficiency in the rectification and distillation columns employed in the concentration of wine and in the solvent recovery column, whereas correlation for extractive distillation (Equation 2) was used only for the ethanol dehydration column. Condenser and reboiler were considered as equilibrium stages for both calculation approaches.

The procedure to determine and include efficiencies in the calculation procedure was an iterative method. First, simulations considering equilibrium stage model were carried out in Aspen Plus® without the addition of efficiency values, which means an efficiency of 100 % (ideal situation). Subsequently, mixture properties were retrieved from the previous simulation and used to calculate the initial values of efficiency through Barros & Wolf efficiency correlation. These efficiencies were inserted in the simulation as Murphree efficiencies and the properties were recalculated, thus obtaining new efficiencies values. This procedure was repeated until the difference between two consecutive efficiency iterations reached a level of tolerance below 1.10^{-4}.

Table 1. Composition of the streams fed to the process

	Wine	Hydrous bioethanol
Water (wt%)	92.0	7.0
Ethanol (wt%)	7.3	93.0
Glycerol (wt%)	0.4	-
Isoamyl alcohol (wt%)	0.2	-
Glucose (wt%)	0.1	-
Mass Flow (t/h)	207.0	16.1

Table 2. Column specifications in bioethanol production process

	Column A	Column A1	Column D	Column B-B1
Number of stages	19	8	6	46
Feed stage	1	1 (WINE) 8 (TOP-A)	1 (REFLUX) 6 (TOP-A1)	22 (PHLEGM-L) 22 (PHLEGM-V)
Sidestream rate (kg/h)	PHLEGM-V 30000 (2^V)	-	-	500 (FUSEL1 - 21^L) 300 (FUSEL2 - 45^L)
Distillate rate (kg/h)	12750			16100

Number in parenthesis shows the withdrawal stage. Superscript denotes the phase, L for liquid and V for vapor.

Table 3. Specifications in the extractive and recovery columns (mass basis)

	Extractive Column	Recovery Column
Number of Stages	32	18
Feed Position	3 (SOLVENT) and 24 (HE)	9
Solvent to Feed Ratio	0.62	-
Reflux Ratio	1.05	0.38
Distillate Rate (kg/h)	15051	-
Bottoms Rate (kg/h)	-	9984

4. Results and Discussion

Efficiency profiles were generated for all columns employed in the complete process and can be seen in Figure 3. It was observed quite different profile for each column. Generally, efficiencies were around 50 % and varied along the columns, except for column A1, which presented constant values.

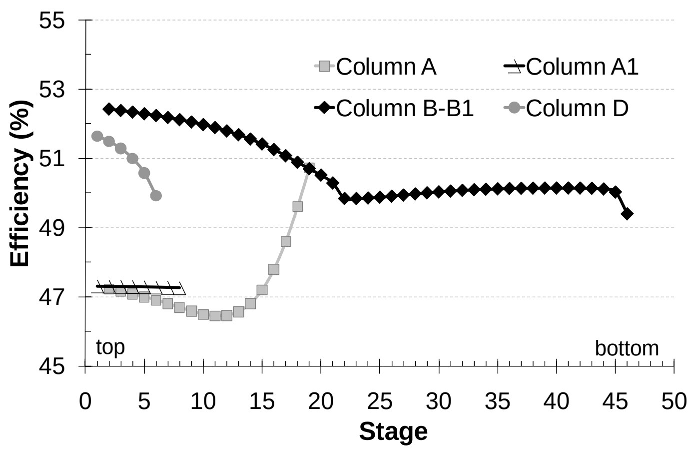

Figure 3. Efficiency profiles obtained in the columns

Results of main streams are compared through Tables 4 and 5. It can be inferred that ethanol contents in hydrous ethanol (HE) and in anhydrous ethanol (AE) are lower when efficiency is taken into account; moreover there is ethanol loss in phlegmasse (PHLEGMAS) and water streams. Stillage and solvent results were the same for both approaches.

Table 4. Stream results for hydrous bioethanol production

	Equilibrium Stage Model (Ideal)			Equilibrium Stage Model with Efficiency		
	STILLAGE	PHLEGMAS	HE	STILLAGE	PHLEGMAS	HE
Temperature (°C)	111.9	107.0	81.7	111.9	105.6	81.7
Mass Flow (kg/h)	175418	14622	16100	175240	14800	16100
Water (wt%)	99.4	99.4	6.8	99.4	98.6	7.6
Glucose (wt%)	0.1	-	-	0.1	-	-
Ethanol (wt%)	-	-	93.2	-	0.1	92.4
Glycerol (wt%)	0.5	-	-	0.5	-	-
Isoamyl alcohol (wt%)	-	0.6	-	-	1.3	-

Table 5. Stream results for anhydrous bioethanol production

	Equilibrium Stage Model (Ideal)			Equilibrium Stage Model with Efficiency		
	AE	SOLVENT	WATER	AE	SOLVENT	WATER
Temperature (°C)	78.3	110	83.5	78.4	110	82.0
Pressure (bar)	1.013	1.013	0.5	1.0	1.0	0.5
Mass Flow kg/hr	15051	9989	1054	15051	9989.0	1054.0
Ethanol (wt%)	99.5	-	-	99.4	-	1.3
Water (wt%)	0.5	-	99.6	0.6	-	98.5
Ethylene glycol (wt%)	-	100	0.4	-	100	0.1

Comparison of temperature profiles in column B-B1 is illustrated in Figure 4. This column was chosen since it has a larger number of stages and, as a result, it is the most influenced column in this process, concerned with the objectives of this work. It was observed that the curves significantly detach from each other between stages 11 and 31, besides the fact that equilibrium stage model (EQ) presents the highest temperature values. This fact can be explained by the assumption that there is enough contact time between the phases to achieve thermal equilibrium. Another observation is that EQ is more sensible to column operation, since the profile presents a disturbance in the feed position (stage 22).

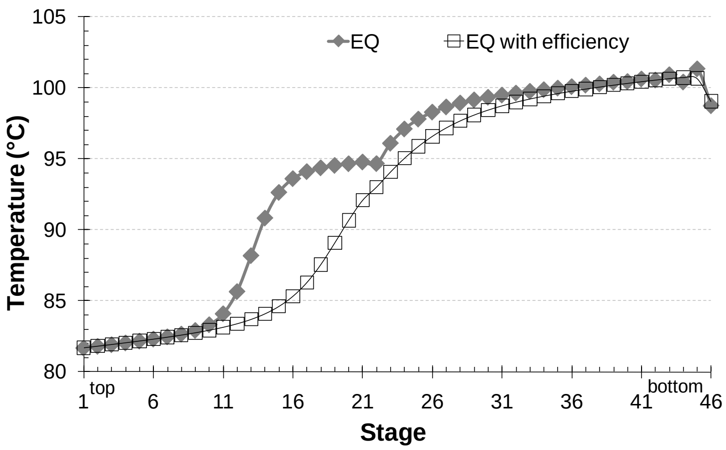

Figure 4. Temperature profile for column B-B1

Temperature profile is also shown for the extractive column in Figure 5. Similarly to column B-B1, curves are coincident in the top and bottom stages. There is also a disturbance in the solvent feed position (stage 24).

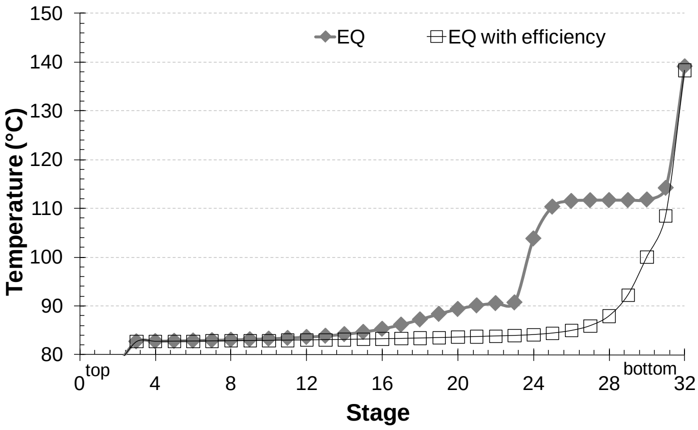

Figure 5. Temperature profile for the extractive column (EC)

Finally, energy requirements for concentration and dehydration processes were evaluated. The first process demanded 26.82 and 26.95 Gcal/h for EQ and EQ with efficiency, respectively. The dehydration process required 3.87 and 3.88 Gcal/h. Therefore, differences in the required energies were not considerable between the calculation methods. However, energy requirements in the concentration process revealed to be significantly higher than in dehydration. Larger flows are the main responsible for this difference.

5. Conclusions

This work has shown the complete separation process in the anhydrous bioethanol production. This is an important step in the product production with a significant impact on the costs. Contrasting to other published works, this study considered other components in wine composition as well as all columns included in the process. Solvent recovery column is usually disregarded and concentration process is usually simplified using a single column. Therefore, simulations were more complex and detailed so that a deeper study can be carried out.

This work proposes a methodology to include efficiency in column calculations performed by a commercial simulator. The introduction of efficiencies reduces the consequences of the idealized assumptions of equilibrium stage model. In the simulated process, efficiencies varied along the columns, oscillating around 50 %. Results also showed significant differences in respect to stream results and temperature profiles when both approaches were compared; however energy requirements were not so influenced by the inclusion of efficiency. In addition, concentration process revealed to be the main responsible for energy demand in the separation step for anhydrous bioethanol production process, particularly due to the large flows involved.

Acknowledgements

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