Simulation and improvement of a typical industrial unity for bioethanol distillation

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Introduction

Besides its use as a renewable energy source, bioethanol has a series of applications as raw material in other industrial branches, such as the chemical, pharmaceutical, cosmetics and beverage industries. Such a larger spectrum of possible uses requires a better control of the product quality and improvements in the production process, even in the case of producing first generation bioethanol, considered as an already mature process in the industrial scale. Ethanol distillation is a topic extensively explored in the scientific literature. Despite this fact, the majority of the published works is focused on finding new possibilities for bioethanol dehydration or for energy saving, without taking into account the influence of the minor compounds on the distillation performance. Considering the important influence of such minor compounds on the performance of industrial distillation unities and the existence, nowadays, of very powerful simulation tools, the absence of this kind of investigation is surprising and limits the possibilities of improving the industrial process of bioethanol concentration and purification.

Results and Conclusions

Considering our prior experience with simulation tools for investigating the concentration and purification of complex multicomponent mixtures, this work aims to reproduce, by computer simulation, a typical installation for bioethanol distillation and the validation of this approach against experimental data collected in a sugar mill operating in São Paulo State (Santa Adélia, Jaboticabal, SP). This research also involved the investigation of the distillation behavior of the main congeners present in fermented must, taking into account their relative volatility in relation to ethanol and analyzing their profiles along the distillation columns. Finally, on the basis of the validated simulation results, new and alternative configurations of industrial equipments can be tested for producing bioethanol with higher quality (neutral alcohol) and lower energy consumption, in both cases taking into account the presence of the main congeners. For this purpose, 20 samples points were installed in the industrial column system of the above mentioned sugar mill and the corresponding samples collected along the last season, also including samples of wine and fusel oil. These samples were analyzed by gas chromatography. Additional information on the operational conditions (streams, temperatures and pressures) were also collected. The Aspen Plus simulator was used for simulating this industrial installation that is composed of five columns with a total of 86 trays. The wine was fed into the column system with a flow rate of 100 m^3/h, a temperature within the range 90-94 °C and around 6 GL of ethanol content, being concentrated to approximately 92.6 % by weight. As waste or byproduct of this system the following streams were withdrawn: stillage, with no more than 0.04 wt% of ethanol, mainly used for fertirrigation; flegmass containing practically only water and used as wash water or for irrigation as well, and fusel oil, an important byproduct of the bioethanol distillation process, mainly composed of active amyl and isoamyl alcohol. Nowadays, the main destination of this byproduct is the cosmetic and fine chemicals industries.

The results showed that the Aspen Plus simulator is able to reproduce with good accuracy the industrial behavior of the main components and of the temperature profiles. The simulated and experimental values for water and ethanol mass fractions and for the tray temperatures have a good agreement from a qualitative as well as a quantitative point of view. For the congeners, the experimental and the corresponding simulated values always have the same order of magnitude, even in the case of components present in very low mass fractions. Nevertheless, in case of some minor components, the relative deviations were higher, attaining values around 60%. However, the trends observed for these components in the simulation results followed those obtained for the same components along the industrial distillation columns. The simulation results can be considered as a reliable estimate of their distillation behavior and of their dependence on the operational conditions and equipment design. The relative volatility results showed a high influence of the ethanol content on the behavior of the congeners, allowing their classification in three categories: *light components* (aldehydes, ketones, esters) whose volatilities are higher than the ethanol volatility, so that these components may contaminate significantly the bioethanol stream; *heavy components* (organic acids) whose volatilities are lower than ethanol´s. These components are easily eliminated from de processes via columns´ bottom products; and *components of intermediate volatility* (higher alcohols) whose volatility depend on the ethanol concentration. In diluted ethanol solutions these components are more volatile than ethanol and the opposite occurs in concentrated ethanol solutions. For this reason these components concentrate in intermediate regions of the columns, requiring their withdrawal by a sidestream.

It was possible to conclude that the Aspen Plus simulator is an excellent tool for improving the current first generation ethanol production and for investigating some alternative equipment configurations able to produce bioethanol with higher quality. In the first case, the influence of minor components in the energy consumption of a double-effect system with split feed of wine was studied, presenting a reduction from 1.78 to 1.19 kg of steam/L hydrated alcohol, in comparison to the traditional process. In the second case, the neutral alcohol production was investigated. Neutral alcohol is a hydrated bioethanol with high purity used in the beverage and fine chemical industries and produced using the biofuel as the raw material. In this case our results showed a large influence of the congeners, since it was necessary the use of further three columns (hydroselection, rectification and demethylation) in order to reach the required quality standard.

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