



Research paper

Simulation and energy analysis of the ABE fermentation integrated with gas stripping



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ARTICLE INFO

Keywords:

Bio-butanol
 ABE fermentation
 Integrated product recovery
 Gas stripping
 Inhibitors removal
 Process intensification

ABSTRACT

The production of acetone, n-butanol and ethanol (ABE) by fermentation has recently gained renewed attention to produce fuels and chemicals from renewable resources.

The main problem associated with the ABE fermentation is the self-inhibition of the process due to butanol toxicity to the culture. The use of a separation method, which enables selective removal of toxic components from the fermentation broth, may contribute to improve the economics of such process.

This work concerns the recovery of butanol from a batch fermenter, in which the ABE mixture is recovered from the broth by means of gas stripping. The aim of this work is to compare the performances of the integrated fermentation-gas stripping process with those of a conventional batch fermenter. For this purpose, both processes have been modeled and their energy requirements have been determined by means of an energy analysis. Results suggest that the continuous product removal from the fermenter allows to reduce the fermentation time by 50%. Therefore, the process productivity is almost double. At the same time, the total specific energy requirement for the integrated recovery process is almost three times greater than that of the traditional batch process. This is essentially due to the duty required at the condenser for products recovery from the gas stream, as a result of the low concentration of ABE in the recovered stream. Therefore, the application of an integrated recovery process allows to increase the process productivity, but at the expense of an increase in the whole process energy demand.

1. Introduction

The increasing greenhouse gas emissions and the resulting global climate change, joined with a growing world population, are key challenges that are leading to an increased interest in processes able to produce fuels and chemicals from alternative, renewable resources [1].

Butanol is an important commodity chemical and an attractive biofuel, which shows several advantages over ethanol [2]. It can be produced through the Acetone-Butanol-Ethanol (ABE) fermentation by clostridia. However, the fermentation is limited by product inhibition, especially due to butanol, and only 22 g L^{-1} of total fermentation products with a butanol concentration below 13 g L^{-1} are typically obtained in the bioreactor during a batch process [3].

Therefore, the ABE fermentation is characterized by high process costs, due to the large volumes required and the downstream product recovery from dilute broths, usually performed by distillation.

The application of integrated recovery techniques that remove butanol from the broth during fermentation represents a viable solution to solve the problems related to the ABE fermentation and to increase the

profitability of the process [4]. In fact, product recovery reduces the effects of product inhibition and allows increasing the process productivity. The operating costs for product recovery are expected to decrease for higher concentrations of ABE in the mixture to be treated.

In an integrated process, products can be separated from the fermentation broth either within the reactor or by circulating the broth through an external separation unit. These two techniques are referred to as *in-situ* and *ex-situ*, respectively [5].

The most mature product removal techniques include gas stripping, solvent extraction, adsorption, vacuum fermentation, pervaporation and perstraction [6].

Gas stripping shows several advantages over other techniques. It is simple to operate and scale-up, it does not require expensive equipment, it does not remove nutrients and intermediates from the broth and it is not harmful to the fermentation microorganism [7]. Several literature works reported the effect of butanol titer in the broth on the stripping process. In this respect, Xue et al. [8] reported that it is necessary to conduct gas stripping at a butanol concentration above 8 g L^{-1} in the feed solution in order to obtain a condensate with a

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butanol titer above its solubility in water, which results in phase separation.

The effects of application of *in-situ* gas stripping on the ABE fermentation have been widely studied, demonstrating the reduction of product toxicity and the resulting improvements in productivity [9].

However, only a few papers appeared dealing with the energy demand associated with this technique. Oudshoorn et al. [10] reported an energy demand in the range of 14–31 MJ kg⁻¹ of produced butanol considering a steady-state process for the separation of a water-butanol binary mixture. Groot et al. [11] considered a two-column system, neglecting the complete separation of acetone and ethanol, obtaining an energy requirement of 21 MJ kg⁻¹ of ABE. Outram et al. [12] compared different *in-situ* product recovery techniques for the separation of acetone, butanol and ethanol from a batch reactor. However, they adopted a simplified representation of the fermenter that was modeled as a stoichiometric, continuous, steady-state reactor. The continuous stream from the fermenter was assumed to represent the desired conditions in the reactor and the fermentation broth was not recycled to the fermenter after the *in-situ* recovery had been applied.

In this work, the effect of the integrated recovery by gas stripping on the whole ABE production process has been studied.

Dynamic simulations of the batch fermentation have been performed in order to investigate the beneficial effect of product removal on the process productivity and to compute the actual concentration levels of the stream sent to the stripping column. Process simulations have allowed to assess the effectiveness of the integrated product recovery technique and the overall energy demand. The integrated process has been finally compared with a traditional batch fermentation, both followed by downstream fractionation of the fermentation products, in order to investigate the potential advantages of process intensification.

2. Thermodynamic framework

Thermodynamics plays an important role in process simulation, allowing to properly describe the phase equilibrium conditions involved in the process under study. The ABE mixture contains many polar compounds and, thus, shows a strong non-ideal behavior, with components pairs also forming azeotropic systems. In addition to this, butanol and water exhibit a miscibility gap, whose correct representation is fundamental for the proper description of the separation process. Therefore, the thermodynamic model must be able to properly describe both Vapor-Liquid Equilibrium (VLE) and Liquid-Liquid Equilibrium (LLE) conditions.

Considering the non-ideal behavior of the system under study, an indirect γ/ϕ method (NRTL-RK) has been chosen in this work for its thermodynamic characterization [13]. It is based on the Non-Random Two-Liquid (NRTL) model [14] and on the Redlich-Kwong (RK) Equation of State (EoS) [15] for the calculation, respectively, of the activity coefficient in the liquid phase and of the fugacity coefficient in the vapor phase. The considered components have been only those effectively removed from the broth, namely acetone, butanol, ethanol, water, and the stripping agent, nitrogen. Firstly, the capability of the model to reproduce phase equilibria using default parameters implemented in the Aspen Plus[®] process simulator has been checked. Then, the model parameters have been regressed to improve model predictions, making use of many binary and ternary VLE and LLE data available in the literature [16]. Nitrogen has been treated as a Henry component and its Henry's law constants have been kept equal to default values. The regressed parameters (reported in Table 1, where acetone, butanol, ethanol and water are denoted by A, B, E and W, respectively) have been implemented in Aspen Plus[®] [17], chosen for the simulation of the distillation process aimed at recovering acetone, ethanol and butanol downstream of the fermentation process. Those concerning the ethanol-butanol and the ethanol-water pairs are not reported in Table 1 because the parameters available in the simulator

Table 1
Regressed parameters for the NRTL-RK thermodynamic model.

i	A	A	A	B
j	W	B	E	W
a _{ij}	-1.6803	3.9225	-2.2512	-2.0447
a _{ji}	4.9929	-3.2661	2.3301	4.2834
b _{ij}	860.74	-1273.33	879.45	980.98
b _{ji}	-1078.63	1196.83	-666.71	-239.15
α	0.5149	0.3000	0.8006	0.4454

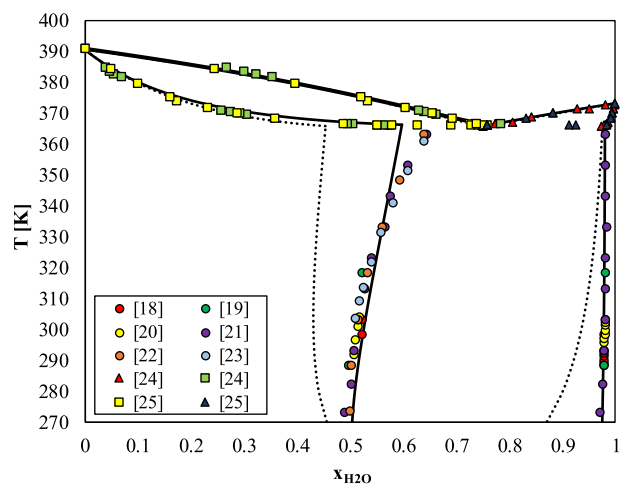


Fig. 1. Comparison between VLE and LLE experimental data [18–25] for the system water-butanol (P = 101 kPa) and prediction by the Aspen Plus[®] [17] NRTL-RK model with default (dotted line) and regressed (solid line) parameters. (For interpretation of the colours in the figure legend, the reader is referred to the Web version of this article.)

have been used for them, being already suitable for satisfactorily reproducing the experimental data.

Fig. 1 represents the temperature-composition diagram for the system water-butanol at 101 kPa. The comparison with the experimental data [18–25] shows a better agreement with the predictions by the proposed model rather than with those by the default model, especially in the LLE region.

The model has been also applied to the ternary systems acetone-water-butanol and ethanol-water-butanol and validated by comparison with the experimental data available in the literature. Results are illustrated in the ternary diagrams shown in Fig. 2 for the system with acetone and in Fig. 3 for the system with ethanol.

3. Process description

In this work, the classic batch fermentation process has been compared with an alternative process solution, which involves a gas stripping operation aimed at removing the fermentation products from the broth in order to reduce inhibition. As reported in the literature, either nitrogen or the fermentation gases (i.e., CO₂ and H₂) can be used for this purpose. However, the use of CO₂ can alter the pH of the fermentation broth, which is a parameter of paramount importance for the stability of the fermentation. Therefore, nitrogen has been considered as stripping agent and an *ex-situ* removal of the fermentation products has been preferred to an *in-situ* one, in order to reach higher performances in a multi-stage rather than in a single-stage unit and without disturbing the fermentation.

Fig. 4 shows the scheme of the integrated process. The fermentation broth is withdrawn from the fermenter and fed to the stripping column at a time when the microorganism starts to be inhibited by the fermentation products. The fermentation broth depleted from the

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