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Simulation and Optimization of the Vacuum Extractive Fermentation Coupled to an Absorption Column for Bioethanol Production Using a High Biomass Concentration

Lia M. Cohen[1*], Henderson I.Quintero[1], Ruben Ramirez[1], Rubens Maciel Filho[1], Daniel. I. P. Atala[2]

[1] Laboratory of Optimization, Design and Advanced Control. Department of Chemical Processes. School of Chemical Engineering. P.O. Box 6066, 13083-970, Campinas-SP, Brazil. Liacohen_0770@hotmail.com
[2] Sugar Cane Technology Center, Brazil.

The ethyl alcohol has positive characteristics for being used as fuel in large scale: relatively low cost, less polluters and can be produced from renewable matrix by fermentation of vegetable source products. By means of process simulation using ASPEN PLUS® V.7, it was evaluated a configuration based on the extractive fermentation vacuum concept coupled to an adsorption column, in which, the alcohol is extracted from fermentation environment while it is produced, as a result, a more productive process is obtained due to a decrease in the inhibition effect on the microorganism caused by the ethanol and at the same time, this configuration allows using a more concentrated must. It was found that the proposed configuration provides a bigger production and recovery of the ethanol contributing to the improvement and intensification of the process.

1. Introduction

The interest in biotechnology-based production of fuels tends to augment with the concern about exhaustion of fossil fuel and the increase in their price. One the world's largest ethanol producers, Brazil has been using sugarcane as raw material for large scale bioethanol production for more than 30 years (Goldemberg, 2007) also the sugar cane industry keeps the greatest commercial energy production in the world with ethanol and the almost complete use of sugar cane bagasse as fuel.
Nowadays there are many minor industrial problems associated with ethanol fermentation processes to be solved, when optimal operation is the target. One of them is the lack of the processes robustness in the presence of fluctuations in operational conditions, which leads to changes in the kinetics behavior, with impact on yield, productivity and conversion. The operation of the alcoholic fermentation process in a continuous mode is desirable, since higher productivity, improved yields and better process control are attained, as well as a low ethanol concentration in the wine due to

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low concentration of substrate used in this process. These conditions are necessary since conventional alcoholic fermentation is a typical inhibitory process, with cells growth rate affected by cellular, substrate and product concentration (Rivera et al, 2006).
The extraction of ethanol is desirable to decrease inhibitory effects over the yeast cells, this is possible using a process in which the ethanol is produced and removed simultaneously through a vacuum flash chamber, also the alcoholic vapor produced in this process contains considerable ethanol concentration so the process is coupled to an absorption column to extract the alcohol using water as solvent.

2. Simulation of the vacuum extractive fermentation coupled to an absorption column for bioethanol production

In order to define the best operating conditions of the vacuum extractive fermentation process, which allow significant reduction on energy consumption as well as on ethanol and sugar losses, the main parameters of the flash chamber (pressure and temperature) and the amount of wine recycled to the reactor were carefully evaluated through several case studies. The evaluated parameters define the degree of phase separation in the flash chamber, and therefore the amount of ethanol recovered in the system. This analysis is of crucial importance on the current development stage of the technology. The results of the optimum configuration of the extractive fermentation coupled with a flash chamber are then compared to those obtained in the conventional fermentation process employed in the Brazilian ethanol industry.
Fermentation reactions mainly comprise sucrose hydrolysis producing glucose and fructose (equation 1) and reduction of sugars into ethanol and carbon dioxide (equation 2). The conversion for the first one is 99% and for the second one is 99.5 %. Also, glycerol, succínic acid, acetic acid and isoamyl alcohol are formed as byproducts as shown in equations 3, 4, 5 and 6 (Eijsberg, 2006).

$$C_{12}H_{22}O_{11} + H_2O \longrightarrow 2C_6H_{12}O_6 \quad (1)$$

$$C_6H_{12}O_6 \longrightarrow 2C_2H_5OH + 2CO_2 \quad (2)$$

$$Glycerol:\ C_6H_{12}O_6 + 4H^+ \longrightarrow 2C_3H_8O_3 \quad (3)$$

$$Succinic\ Acid:\ C_6H_{12}O_6 + 2H_2O \longrightarrow C_4H_6O_4 + 2CO_2 + 10H^+ + 10e^- \quad (4)$$

$$Acetic\ Acid:\ C_6H_{12}O_6 + 2H_2O \longrightarrow 2C_2H_4O_2 + 2CO_2 + 8H^+ + 8e^- \quad (5)$$

$$Isoamyl\ Alc:\ C_6H_{12}O_6 \longrightarrow 0{,}79C_5H_{12}O + 2{,}02CO_2 + 1{,}15H_2O + 0{,}15H^+ 0{,}15e^- \quad (6)$$

In the proposed process, the ethanol produced during fermentation reactions is continuously removed from the fermentation media, allowing the use of higher concentration substrates (about 400 g/L) and maintaining the ethanol content into the

reactor at low levels (about 8 wt%). The product is continuously removed from the reactor. A purge is made to remove low-volatile products before being fed to a vacuum flash chamber where an ethanol-rich vapor phase and a liquid phase are formed. The liquid phase is recycled to the reactor while the vapor phase, which contains the wine, is sent to the purification step in the absorption column using water as a liquid absorber to separate the alcohol. The wine produced in the flash chamber contains approximately 30 wt% ethanol; as a consequence, less energy is required to produce hydrous ethanol. The flowsheet of the extractive fermentation process coupled with a vacuum flash chamber and the absorption column is shown in the figure 1.

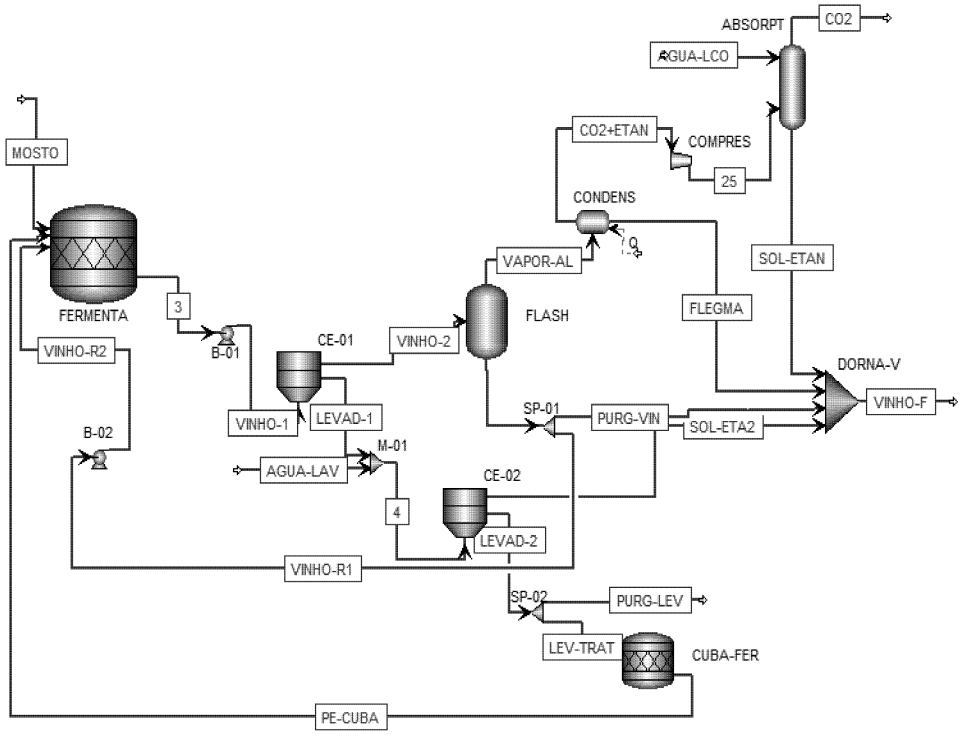

Figure 1: Flowsheet of the vacuum extractive fermentation process

The main objective of the fermentation process is to obtain high concentration of ethanol in the wine, which is desirable to achieve low energy consumption on the subsequent distillation stage as well as a complete consumption of sugars in the fermentation media.

3. Results and Discussion

ASPEN PLUS V7.1 software was used to simulate the process configuration for vacuum extractive fermentation proposed in this work. NRTL thermodynamic model

was chosen to calculate the activity coefficient on the liquid phase because of the good performance to represent highly non-ideal mixtures.
The aim of this work was to find the optimal conditions in the unit operations of the configuration to produce ethanol in greater quantity and with higher purity. Operating pressure and temperature in the flash unit separation coupled to vacuum pump were modified; these have direct influence on the ethanol and CO_2 mass fluxes in the output streams of unit. By sensitivity analyses was see the variables behavior and are shown in the figures 2 and 3.

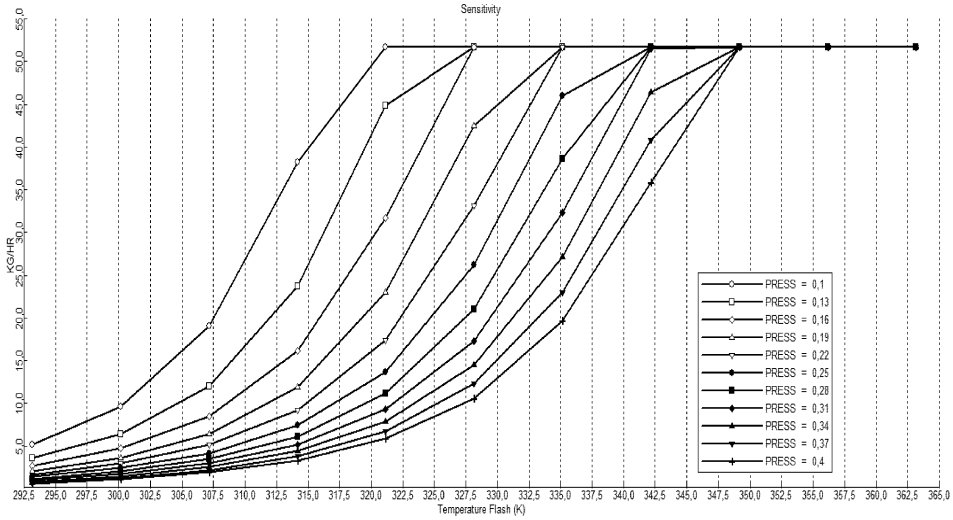

Figure 2: Ethanol mass flow variation in the current VAP-ALC with temperature and pressure changes in the vacuum flash unit

By the sensitivity analysis done on the ethanol content in the current VAP-ALC can be seen that the optimum ranges of operation are pressure values between 0.1 and 0.2 atm and temperatures between 320 and 323 K, because in these ranges the mass flow of ethanol and carbon dioxide in the stream reaches a maximum of ethanol in the vapor phase Figure 3 shows that ranges of temperature and pressure in the VIN-RECT stream were optimal. Absorption unit was optimized by the analyses of the influence of variation of water flow and the number of stages on the output currents CO_2 and SOL-ETAN.

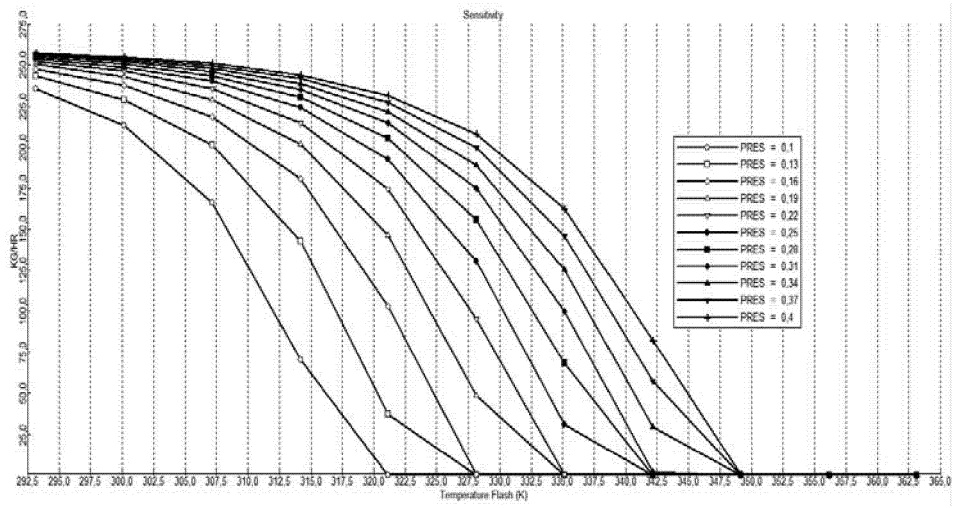

Figure 3: Ethanol mass flow variation in the current VIN-RECT with temperature and pressure changes in the vacuum flash unit

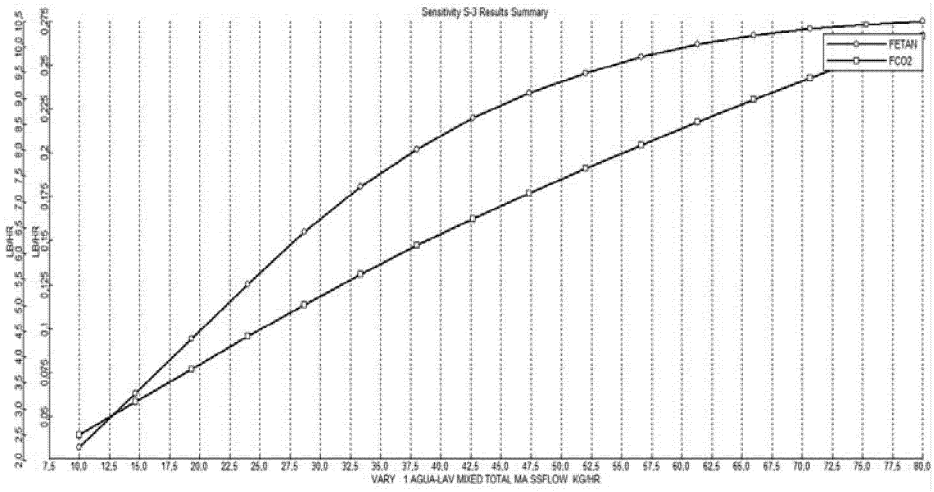

Figure 4: Ethanol and CO_2 flow variation in the current SOL-ALC with water flow changes in the absorption unit

The figure 4 shows that an increase in the flow of current AGUA-LCO represents an increase in the amount of ethanol recovered, we can also see that the amount of ethanol contained in the SOL-ETAN stream also increases and contains insignificant amounts of CO_2, however it chosen to use less than 100 lb/h of water since this is an important resource and reduces costs in the operation of distillation. It was also done the sensitivity analysis to determine the optimal number of stages for the best separation. This analysis showed that the variation is minimal and therefore was use the least amount of stages in the simulation ensuring a good separation of components.

Table 1: Streams total mass flows and bioethanol recovery for each streams

Stream	Total mass flow (kg/h)	Ethanol mass flow (kg/h)
MOSTO	1261,05	0,0
LEV	55,56	0,0
VINHO-1	1316,61	67,49
VINHO-2	1261,05	67,23
VINHO-R1	761,02	14,96
PUR-VIN	190,25	3,74
VAPOR-ALC	276,25	48,47
SOL-ETAN	21,03	2,26
FLEGMA	250,23	42,95
VINHO-F	461,51	48,95

Compared to the conventional process, the configuration proposed in this work involves a compressor and vaporizator unit, which means more energetic requirements. Nevertheless the very good results regardinng to the ethanol separation (reaching up to 80% of ethanol recovered) compensates the extra energtic spentsas it is shown in the table 1.

4. Conclusions

The vacuum extractive fermentation process proposed reaches higher levels of ethanol production than the conventional fermentation process. It was found that the configuration used , and the recycle of cells and ethanol to the reactor, lets to reache a maximum level of ethanol recovery at all stages. That configuration allows to work with more concentrated must without suffering the inhibitory effect of ethanol on yeast. Also the wine produced in this process contains higher ethanol concentration, thus the energy consumptiom is decrased in the further distillation stage.

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