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Simulation of Furfural Production Process for Revamping with Ethanol Technology from Lignocellulosic Residuals

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Evaluation of alternatives for the intensification and revamping of sugar cane industrial facilities is necessary for the competitive development of this production process. Bagasse is a by-product of cane sugar production, used for heat cogeneration, and for furfural, boards and ethanol production from lignocellullosic residuals. The furfural hydrolysis stage coincides with the acidic pretreatment stage of ethanol technology. From previous obtained results in ethanol technology from lignocellullosic residuals (Mesa, 2009) and by changing different operation conditions of the furfural hydrolysis step, applying smaller reaction times (Morales, 2009), usable residual and condensed furfural with an appropriate composition could be obtained. The objective of this study was to carry out the simulation of the furfural production process for revamping ethanol technology of lignocellulosic residuals using the ASPEN PLUS software. Mass and energy balances were determined in the acid hydrolysis stages of the bagasse and furfural distillation units. Different economic and technical alternatives were investigated and analyzed into detail by global process simulation, both for the batch reaction unit for furfural production, as for the continuous distillation for its purification. Different suggestions for reanimation of furfural plants exist for revamping with ethanol technology from lignocellullosic residuals. For them it is necessary to take advantage of new installed production capacities and to adapt power availability of raw materials and carriers in the cane sugar production process.

1. Introduction

The companies doesn't should to consider definitively installed in a market, in a certain technology in order to prevail in a competitive world as the present and to even survive. Every time that are desired to incorporate cleaner technologies, modernization, reordering or revamping industrial installation must be concentrated in three main goals for the investments in a developing country which are based on: increase the capacity of the plant with a stable quality of the product and diminution of consumptions, especially imported, decrease the return time of investment destined for plants modernization and increase the installation availability.

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Bagasse constitutes the greater by-product of Sugar Industry and it is used essentially for heat cogeneration, and for animal food, furfural, boards and more recent ethanol production from lignocellullosic residuals.
The furfural hydrolysis stage coincides with the acidic pretreatment stage of ethanol technology. From previous obtained results in ethanol technology from lignocellullosic residuals (Mesa, 2009) and by changing different operation conditions of the furfural hydrolysis step, applying smaller reaction times (Morales, 2009), usable residual and condensed furfural with an appropriate composition could be obtained.
The objective of this work consists: evaluate the impact of revamping of furfural production with the best obtained results of ethanol technology from lignocellullosic residuals using ASPEN PLUS software.

2. General Considerations on Use Biomass like Product Source of High Added Value

Bagasse of sugar cane is a residual of sugar production from sugar cane and is great potential for ethanol technology from lignocellullosic residual. Given the resistance of lignocellulosic matrix to enzyme attack is necessary to consider a system of previous pre-treatment. The best form to evaluate the quality of this in lignocellulosic material will be without a doubt the effectiveness of enzymatic hydrolysis in standardized conditions.
For specific case of sugar cane bagasse several systems of pre-treatment have been used. In particular the pre-treatment has been used with better results organosolv in two stages (acid and another basic one) as well as an analysis of cost production for different alternatives from treatment with two stages (Mesa et al., 2009; González et al., 2009).
The pre-treatment in 2 stages was evaluated. First (acid) to separate xylano fraction of bagasse and to obtain pentose for ethanol or other uses. Second (organosolv) to separate lignin (good quality) and to increase efficiency of enzymatic hydrolysis (HE). The main results obtained summary that:

- The use of H_2SO_4 shows better results in analyzed experimental region on the parameters answers studied.
- The use of two stages means an increase in all results as well as an increase in number of equipment and value of investment, reason why an analysis of economic alternatives technical prevails.
- Require changes in operation conductions of acid pre-treatment in agreement with the end that are wanted to use pentoses for example: in furfural production, xylytol, ethanol, For case of furfural obtaining: Temperature 175-185^oC; Solid relation - liquid (1/1).
- It is required to deepen in use of recovered lignin and in solid residual of HE.

The furfural technology obtaining includes hydrolysis and refinement process. One forms as a result of pentoses decomposition. Kinetic of decomposition of xylose during a heating in ampoules in aqueous solution to temperature between 140 ^oC and 220 ^oC. In this case the reaction of pentose decomposition is catalyzed by own formed acid products in process.

3. Materials and Methods

The tasks of investigation are developed applying tools of process analysis and simulation so that allow obtaining an integral analysis as it is described next:

1. Description and diagnosis of bagasse hydrolysis stage and furfural plant.
2. Proposal and evaluation of operational changes in bagasse hydrolysis stage from the best results obtained in the technology of bagasse bio-ethanol.
3. Simulation of hydrolysis and distillation stage with the data of design of installed equipment from obtained results of revamping in bagasse hydrolysis stage.
4. Economic analysis of revamping impact in hydrolysis and distillation stage for reanimation of furfural plant.

1.1.1. Conditions in investigation tasks

1. The furfural hydrolysis stage coincides with the first acid stage of pre-treatment of ethanol technology of lignocellulosic residual. Therefore it is feasible to analyze acid hydrolysis of furfural preliminarily from best obtained results of ethanol technology of lignocellulosic residues (Mesa, 2008) and to change operational conditions with smaller condensate and reaction time that allow obtaining a usable residual, of furfural with a suitable composition.
2. The best obtained results on pilot scale are described in Table 1. Was obtained a condensate with 2% furfural when evaluating experimentally.

Table 1: Impact of condition one of first stage of pre-treatment in xylose recovered. Base: 100 grams of dry bagasse.

Temp	Time Min.	% Acid	S/L	Reactor	Xylose End	% Recovered Potential	% Recovered Real
120-130	40	4	4/1	Laborat	6,755*	72,89	72,89
120-130	40	4	4/1	Pilot	7,626	69,50	42,51
175-185	40	1	1/1	Pilot	12,547	49,81	4,52

3. The following considerations are taken into account for simulation of stages of furfural production process from obtained results of revamping proposal and with the data of design of installed equipment in the Figure 1 and 2 are represented two stage of this process:

Bagasse hydrolysis stage. Discontinuous reactor. Components: Bagasse, H_2SO_4, xylose, furfural, water.

$T_{reactor}$ = 175°C; 9 P = 1 atm; Valid phases: Steam-Liquid; $t_{reaction}$ = 2400 s;

Continuous feed: Steam; Reaction: Xylose conversion; Used method: VANL-HOC

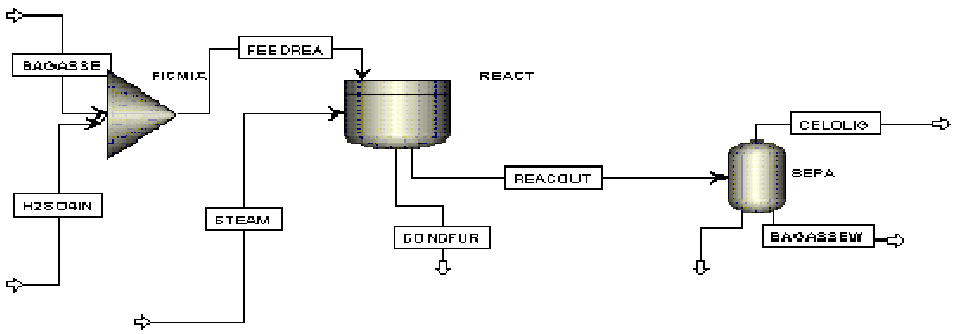

Figure 1: Diagram of bagasse hydrolysis stage

Furfural distillation stage. Used method: UNIF-LL; UNIFAC
Components: Furfural, water.
<u>Column 1</u>
Number of stages = 30; Feed = 3 Total condenser; Valid phases: Vapor-Liquid;
Reflux ratio (mass) = 5; Distillate to feed ratio = 0.08
<u>Column 2</u>
Number of stages = 24; Total condenser; Valid phases: Vapor-Liquid-Liquid; Convergence: Azeotropic; Reflux ratio (mass) = 9; Distillate to feed ratio = 0.08; Decanter: Fraction of decanter liquid flow returned to column = 1; $T_{subcooled}$ = 50 ^oC

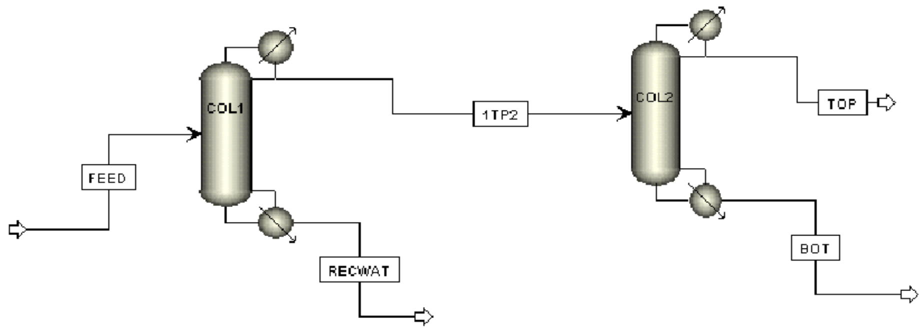

Figure 2: Diagram of furfural distillation stage

4. Two variants are valued using three and two installed reactors for economic analysis from analysis of all equipment of plant and demand-capacity of raw material (bagasse), The results of mass and energy balance of bagasse hydrolysis and distillation stage are shown in Tables 2 and 3. This results corresponding to main flows of processes as well as the compositions of main components in each stage.
Firstly it is analyzed using maximum capacity of production where 1 digestion is equivalent to use 3 digestors. In each digestor are feed 4 t bagasses with 50% fiber. If one knows is obtained 1 ton of furfural by each 40 ton of bagasse which represents for this conditions 144 ton bagasse/day and each digestor to work a capacity of 4 bagasse digestion and it assumes 6 digestions work turn for 3 work turn day, is possible to

obtain 1, 8 ton furfural waited for in production plant, under the present conditions, without analyzing modification.
However, if impact proposal of revamping in bagasse hydrolysis stage is analyzed under analyzed experimental conditions and as a result of simulation of stages process, it is possible to obtain 1, 37 ton of furfural which favors the awaited final results.

Table 2: Summary of mass and energy balance in the acid hydrolysis stage of bagasse.

Fraction Mass/ Raw	Bagasse	H_2SO_4 in	Feedrea	Steam	Cond Fur	Reacout	Celolig
H_2O	0.2346	0.99	0.242	1	0.7369	0.992	0.992
H_2SO_4	0	0.01	9.90E-05	0	3.69E-05	1.48E-05	1.48E-05
Xylose	0.2966	0	0.2936	0	0.056	0	0
Furfural	0	0	0	0	0.0339	0.00747	0.00747
Sucrose	0.4688	0	0.4641	0	0.1727	4.01E-06	4.01E-06
Ftotal kg/s	0.5555	0.0055	0.5611	0.9461	1.005	7.19E-05	7.19E-05
Ftotal kg/h	1999.8	7999.92	9999.72	3405.96	8938.51	0.2588	0.2588

*Legend: **Bagasse**: Feed bagasse; **H_2SO_4 in**: Feed sulphuric acid; **Feedrea**: Mixture of entrance to reactor; **Steam**: Vapor feed the reactor; **CondFur**: Furfural condensate exit of reactor; **Reacout**: Residual bagasse exit of reactor; **Celolig**: celolignin.*

Table 3 Summary of mass and energy balance in furfural distillation stage.

Fraction Mass/Raw	Feed	1TP2	Recwat	Bot	Top
H_2O	0.98	0.7499	1	0.810	0.0597
Furfural	0.02	0.25	8.64E-10	0.1899	0.9403
Ftotal kg/s	2.4827	0.1986	2.284	0.1827	0.0158
Ftotal kg/h	8938.00	715.037	8222.96	657.835	57.203

*Legend: **Feed**: Furfural condensate feed column 1; **1TP2**: Vapor exit of column 1; **Recwat**: Exit flow column 1; **Bot**: Residual exit flow column 2; **Top**: Furfural exit flow column 2.*

In dependency of power scheme of sugar complex and efficiency it is possible to obtain from a 10-15% of residual bagasse that is used like fuel and source of other productions. In studied company the power scheme this inefficient one therefore requires of later analysis to obtain suitable advantage of bagasse that allows the availabilities and provisions to derivates plants.
For the economic analysis, from: defectation of all the equipment of the plant, and an analysis of demand-capacity of raw material (bagasse). Next in Table 4, economic results of balance and indicators are obtained analyzing the use of 3 digestors and 2 digestors in process production. It is demonstrated that still diminishing the capacity of production by low availability of raw material promising results of economic indicators were obtained justifies the analysis investor for possible reanimation of plant.

Table 4. Main Results obtain with balance and economic indicators.

Variables	Version 3 digesters	Version 2 digesters
Bagasse Consumption (t/d)	144	96
Furfural Production (t/d)	4.11	2.74
VAN ($)	574,025.21	363,927.07
TIR (%)	33	25
PRD (years)	4.5	5

4. Conclusions

From revamping in the conditions of operation of stage acid hydrolysis of furfural production it is possible to obtain: a usable fibrous residual for the stage of enzymatic hydrolysis the ethanol technology of lignocellulose residues and furfural condensate with a suitable composition for the stage of furfural distillation. The simulation of furfural process is obtained using Aspen PLUS 11.1 and promising results are obtained. The technical-economic analysis in furfural plant satisfactory results of economic feasibility for the two analyzed variants are obtained based on the availability of raw material offering to better results the variant of using installed capacity with a PRD of 4.5 years.

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