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Simulation of the Batch Fermentation Stage in the Process to obtain Ethanol from Final Molasse

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The purpose of this study is to develop a general method to obtain a better yield in the alcohol production from molasse. Ethanol fermentation is carried out as a batch process. In practice, variations occur in parameters such as biomass concentration, temperature, and other important variables. For those reasons it is very important to have a strict parameter and process control in order to have proper reaction circumstances. The fundamental parameters of operation are mainly a temperature around 35 ^{o}C and at ambient pressure. The Aspen Plus Software was used for the simulation of the whole batch reactor process. The simulation starts with a rigorous material balance of the reaction. This reaction is globally exothermic, ethanol formation being the main product besides carbon dioxide and biomass as by products, starting from glucose as a standard sugar component, applying urea in low proportions as nitrogen source. In this process Saccharomyse Cereviciae yeast has been used as microorganism. A kinetic study was undertaken taking into account data from an existing factory, as well as data collected from specialized literature for cases not known from direct process measurements. The kinetic constants are obtained from the Monod kinetics, equivalent to the Langmuir Hinshelwood Hougen Watson model, which can given into the Aspen Plus model. The batch reaction time is taken for 16 h in the bioreactor simulation, together with a batch feed time of 8 h. Air has been added continuously, to provide the necessary oxygen source. A sensitivity analysis is carried out in addition to vary parameters like reaction time, and feed flow, to analyze the dependency on ethanol production. This analyze shown an exponential formation in agreement with the Monod Law with a maximum ethanol production in 18 hours, which is close to the real process time at the moment.

1. Process description

The process of producing ethanol from sugar cane molasses has three main stages: substrate preparation, fermentation and distillation, Figure 1. In the first stage the molasses is prepared according to the pre fermentation process necessities for further growth of yeast culture during this stage, maintaining a strict pH control, the number of microorganisms and temperature according with Nielsen, (2003) and Phisalaphong

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.(2006). In the fermentation stage the sugars contained in molasse are transformed into ethanol, controlling again the same parameters: pH, the number of microorganisms and the temperature. The concentration of alcohol in the ferment is about 4.5 GL. This step is followed by distillation. In this operation is obtained an alcoholic concentration of 96.3 ^{o}GL as a final product, this alcohol is called extra fine alcohol.

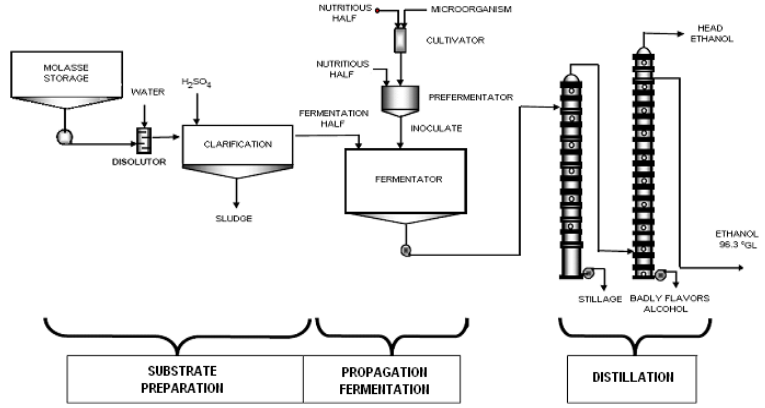

Figure 1: Process Description Flow sheet.

1.1 Simulation of Batch Fermentation Stage

For simulate batch fermentation stage in the process to obtain ethanol from molasse was used Aspen Plus 11 Software (Seider et al, 2004) and (Qin .2009). In the Figure 2 is showed the flow sheet for the stage simulated. At first place it was necessary to make a complete definition of the components involved in this stage such as water, ethanol, carbon dioxide, oxygen, nitrogen, glucose, ammonia and urea as source of Nitrogen and NH_3.

Table 1 Batch fermentation parameters

Parameter	***Value***	***Measurement Unit***
Temperature	35	°C
Pressure	1	atm
Stop value	20	h
Batch feed time	8	h
Down time	2	h
Maximum calculation time	30	h
Time interval between profile points	1	h
Maximum number of profile points	25	-

Table 2 Flash fictitious unit parameters

Parameter	***Value***	***Measurement Unit***
Temperature	35	°C
Pressure	1	atm

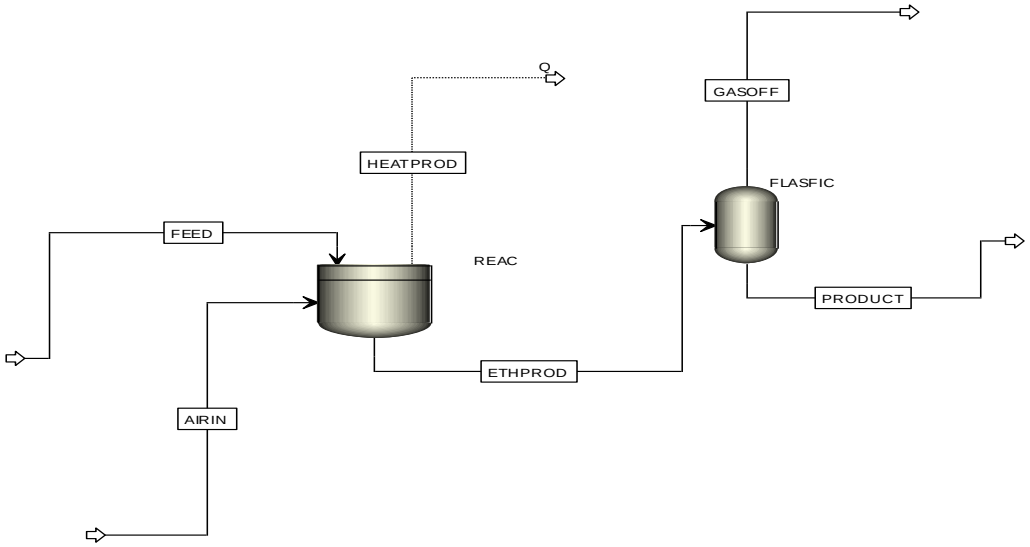

Figure 2: Batch Fermentation scheme using Aspen Plus Software

The VANL-HOC model was selected in the thermodynamics model definition, (www.scribd.com) this method is useful to calculate activity coefficients based on VAN LAAR methods.

1.2 Material Balance

For the simulation it is necessary to carry out a rigorous materials balance, for that was considered the glucose contained in the final molasse as the main substrate.

A few years ago (Raghav et al, 1989), reported the data that appear in Table 3. This data include the kinetic parameters to batch fermentation of molasse using the Saccharomyse Cerevisiae yeast and theses kinetics parameters were used in this paper to simulate the kinetics in extra fine alcohol process. The main results of materials balance are showed in Table 4 and Table 5.

Table 3 Kinetics parameter using Saccharomyse Cerevisiae yeast

Kinetic parameter	***Value***	***Unit***
Specific grow rate μ	0.08	(h^{-1})
Specific ethanol production rate q_p	1.60	(g/g/h)
Specific glucose uptake rate q_s	3.50	(g/g/h)
Overall biomass yield Y x/s	0.023	(g/g)
Final ethanol concentration	65	(g/l)
Overall ethanol yield Y p/s	0.474	(g/g)
Ethanol yield (% of theoretical)	93.0	%

From the overall ethanol yield Y p/s can calculate the grams of ethanol formed by each gram of substrate.

Table 4 Main results of materials balance

Parameter	Value	Unit
Ethanol Formed	85.32	g ethanol/mol glucose
Ethanol Formed	1.855	mol ethanol/mol glucose
Biomass Formed	1.314	g biomass/mol glucose
Biomass Formed	0.01163	mol biomass/mol glucose
Nitrogen IN (Urea)	0.005815	mol
Carbon in Glucose IN	6	mol
Carbon in Urea IN	6	mol
Carbon in Ethanol OUT	3.710	mol
Carbon in Biomass OUT	0.05815	mol
Carbon in Carbon Dioxide OUT	2.1253	mol
Hydrogen in Urea IN	0.02326	mol
Hydrogen in Glucose IN	12	mol
Hydrogen in Ethanol OUT	11.13	mol
Hydrogen in Biomass OUT	0.08141	mol
Hydrogen in Water OUT	0.40589	mol
Oxygen in Glucose IN	6.0	mol
Oxygen in Urea IN	0.005815	mol
Oxygen to suministrate	0.2528	mol

Table 5 Results of materials balance obtain with Aspen Plus.

Mass Flow kg/sec	AIRIN REAC VAPOR	ETHPROD FLASFIC REAC LIQUID	FEED REAC LIQUID	GASOFF FLASFIC VAPOR	PRODUCT FLASFIC LIQUID
H_2O	0	0.777885	2.123054	0.035474	0.742411
Biomass old	0	2.03E-03	5.06E-03	7.73E-07	2.03E-03
Ethanol	0	0.068548	0	7.19E-03	0.0613574
Biomass new	0	8.63E-04	0	3.28E-07	8.63E-04
CO_2	0	0.0789939	0	0.077123	1.87E-03
O_2	0.2445587	0.2126943	0	0.21143	1.26E-03
N_2	0.8054236	0.7322032	0	0.729542	2.66E-03
Glucose	0	0	0.3972818	0	0
Urea	0	1.56E-03	5.06E-03	0	1.56E-03
Total Flow kmol/sec	0.036394	0.079298	0.1201816	0.036528	0.0427705
Total Flow kg/sec	1.049982	1.87478	2.530457	1.06076	0.8140201
Total Flow cum/sec	0.9049601	3.24E-03	2.41E-03	0.922851	8.44E-04

1.3 Reaction Definition

It was considered as principal reaction (Eq.1). Direct reaction is the reaction to transform the glucose present in molasse in presence of nitrogen and oxygen from Urea. Reaction products are ethanol and carbon dioxide (Watt and Sidhu, 2010). A detail of

this case is that the old biomass present in reaction is transformed in new biomass and same occurs with inverse reaction, new biomass is transformed in old biomass.

$$C_6H_{12}O_6 + 0.3769\ O_2 + 0.005814CH_4N_2O \Rightarrow$$
$$0.01163C_5H_7NO_2 + 1.855C_2H_6O_2 + 2.2377CO_2 + 0.4059H_2O$$

2. Sensitivity Analysis

A sensitivity analysis to analyze the dependency on ethanol production is carried out with the variation of parameters like fermentation time and feed flow. This analyze shown an exponential formation in agreement with the Monod Law with a maximum ethanol production in 18 h, which is close to the actual process - Figure 3.

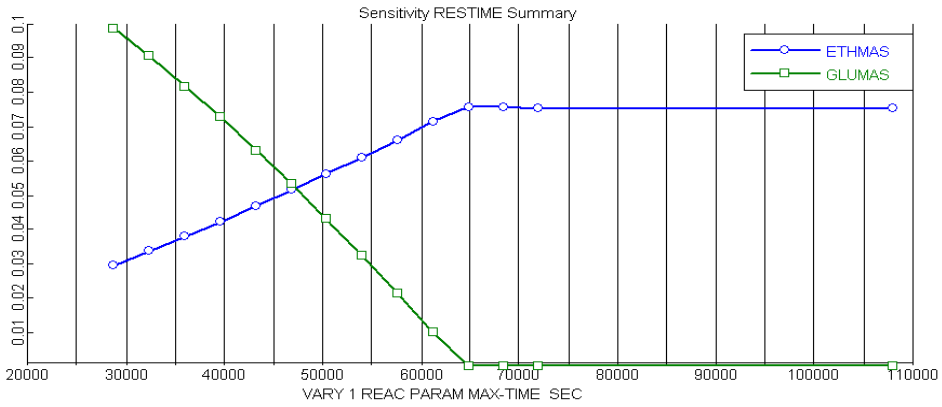

Figure 3: Relations between fermentation time and Ethanol production and Glucose consumption

3. Conclusions

Process simulation of ethanol fermentation stage from final molasse helped to analyze and to have a strict control above the variations that occur in parameters as biomass concentration, temperature. A kinetic study was undertaken employing data from an actual factory, as well as data collected from specialized literature these one in order to supply the data that not known from direct process measurements.

By the simulation is possible have a strict parameter and process control in order to have proper reaction circumstances; for example a sensitivity analysis shown an exponential ethanol formation in agreement with the Monod Law with a maximum ethanol production in 18 h, which is close to the actual process. The fermentation stage simulated represents very well the stage on the industry, final ethanol production obtained by simulation was 68 g/L which is according with the actual process.

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