## SIMULATION OF AN INDUSTRIAL PLANT OF ANHYDROUS ETHANOL PRODUCTION FROM SUGAR CANE JUICE Paper Number: 126848

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# Introduction

Fuel ethanol has become an alternative of renewable energy source, because the less production to medium term of petroleum and contamination that the derivatives from the fossils fuel produce. The process of anhydrous alcohol production reunites to different stages from reaction and separation, which combined and with slight variations can get to produce different ethanol qualities. In this work a detailed study becomes of the process by means of simulation in Aspen Plus v2006. Established down the main operating conditions and different alternatives are evaluated to select the best one in some important stages. The simulated process involves from cane juice preparation for the fermentation to the process of ethanol dehydration, in this last process evaluate two techniques of dehydration, the extractive distillation with glycerol and adsorption by molecular sieves. The restriction of the simulation is the ethanol composition in the bottoms stream of the stripping, rectifying and recovery column, and the ethanol composition in distilled of the column the dehydrator. The results show that the kinetics reaction of glucose fermentation fits the power law of first order and that the process of dehydration of the mixture ethanol-water by extractive distillation with glycerol as separating agent is efficient from the energy consumptions and economic point of view.

# 1. Production process of Fuel Ethanol from Sugar Cane Juice.

The first step in obtaining alcohol fuel is the fermentation process where the sugar content in juices and honey of crops are transformed into alcohol using yeast. Subsequently fermented alcohol becomes a distillation columns where, through a process of evaporation is separated from the compound, obtaining alcohol purest, stillage and fusel oils. The final stage is dehydration, which withdrew water obtaining anhydrous alcohol. The process can be seen in the block flow diagram in Figure 1.

## Fermentation

For the fermentation process used four reactors type stirred tank (CSTR) in series with cascade technology, with recirculation of yeast. It is fed continuously cane juice (14°Brix) to the first fermenter (Cardona, 2006). Likewise, feed crops of *Saccharomyces Cerevisiae* from the vats of reproduction and circulation to maintain cell population levels between 200-300 million cells per milliliter of solution in the fermenter. This fermentative process is under anaerobic conditions at a temperature of 32 to 35°C and a pH of 4.2 to 4.5 (Jacques, 1999).



Figure 1 BFD Anhydrous Ethanol Production Process

## Ethanol Recovery

The wine stripping, the fermentation product, which usually takes on average 7% v/v (Gil, 2006), is pumped into a preheated exchanger plates at a temperature of 80 ° C, then switched to a degassing column, which removes compounds with lower temperature of boiling that ethanol. For obtain ethanol 40-45% v / v (Gil, 2006), the mixture is sent to a Stripping column, which is powered by steam of 45 psig to separate alcohol (Gil, 2006), in the bottoms of the column leaves a byproduct called stillage which will be discussed in later sections. In the ethanol rectification stage, vapors with 40-50% ethanol concentration from the top of the stripping column are sent to a rectifier column (Cardona, 2006). The byproducts from column bottoms are called flemazas.

#### Ethanol Dehydration

The molecular sieves are materials that are characterized by their excellent ability to retain on its surface defined types of chemical species (Gomez, 2007). A key feature in operations involving the action of molecular sieves is that the amount of the substance to rowing-see through the sieve should be low. A synthetic zeolite 3Å type used in the vast majority of dehydrated ethanol, because their pores with a diameter of 3Å, while water molecules have a diameter of 2.8 Å and molecules of ethanol a diameter of 4.4 Å (Gil, 2006). Thus, water molecules are strongly attracted within the pores and the molecules of ethanol passes through a bed without experiencing any attraction (Gil, 2006).

Dehydration alcohol by extractive distillation consist in to add a solvent to the ethanolwater mixture (this mixture is impossible to separate by ordinary distillation) altering the relative volatility of the components and allows separation. But the solvent should be have low volatility, not even be a way evaporate in the column.

## 2. Process Simulation

The NRTL model fits best to equilibrium because the components involved in the process have characteristics of polarity and electrolytes, besides operating conditions in the process is less than 10 bar pressure (Carlson, 1996). The process assumes a pressure drop, which implements pump units, which discharged liquid flows at a pressure of 25 psi, this value was calculated using a heuristic and assumes a head of 20 ft (Seider, 2003).

#### **Fermentation**

The reaction is carried out in four reactors in series CSTR simulated in a module for calculating RCSTR modeling rigorously the reactor, manages kinetic reactions and equilibrium as well as the reactions involving solids. It can provide the kinetics of the reaction in the reactions models. To know the reaction kinetics of glucose fermentation, experimental data were taken at a temperature of  $33^{\circ}$ C and then uses a Integration Method (Fogler, 2001) to determine the rate constant k, which assumes Reaction order of one regarding glucose. Figure 2 shows the Flowsheet Diagram of simulation of fermentation



Figure 2 Flowsheet Diagram of simulation of fermentation

#### **Alcohol Distillation**

Figure 3(a) shows the Flowsheet diagram of the simulation of stripping stage. The stripping column (T-201) is simulated with a distillation column with steam saturated injected directly to a pressure of 45 psig; The Bottoms Stream, where leaves stillage, is used to preheat the feed stream to the stripping column, for this is used a module HeatX where specified temperature output desired in the cold stream in the exchanger (80°C) to separate the more volatile compounds. Figure 3(b) shows the Flowsheet diagram of simulation of rectification and recovery stage.

Much of the ethanol fed into the rectification column, leaves by the distillate with a mass fraction of 95%. In the column specifying a stream of fusel high side that corresponds to a mixture of alcohols rich in propanol and its extraction are performed five stages above the feed stage. On all the columns specifies a Murphree efficiency of 0.68 per stage (Kister, 1990) to adjust the results to reality and get a column size approximate of the industry Distilleries. The pressure drop in the stripping column is considered linear, (estimated by heuristic), with a value of 0,015 atm per stage (Seider, 2003).



Figure 3 Flowsheet Diagram of the Simulation of Ethanol Distillation

#### Ethanol Dehydration

The most used Techniques for alcohol dehydration industry are the extractive distillation and adsorption by molecular sieves. Figure 4(a) shows the Flowsheet diagram of dehydration by extractive distillation. The Feed stream to the dehydration column is a liquid saturated of azeotropic ethanol. When already know the flow rate of glycerol, realize a specification design such that the flow rate of solvent make up mixed with the flow rate of bottoms from the regenerate column are equal to the flow rate calculated above. It is done with the help of the tool Design Spec Flowsheeting option under the Options, there is created a new analysis, specifying the desired flow molar solvent input to the column and varies the flow rate of solvent make up within a consistent interval.



**Figure 4** Flowsheet Diagram of the Simulation of the Dehydration by Extractive Distillation.

The dehydration by adsorption with molecular sieves is a cyclical process of separation, i.e., while the first adsorbs the second regenerates. Consist of two packed columns with zeolites or carbon compounds adsorbents. The bed that is packed in adsorption operates at high pressure of 25 psig while the second screening is carried out the operation of regeneration to a reduced pressure of 26 inches of mercury (Gil, 2006), which is achieved

by combining a condenser and a ring vacuum pump liquid. Figure 4(b) shows the Flowsheet diagram of the simulation process by adsorption molecular sieves.

## 3. Results

With the specifications given in each of the stages of the simulation process of producing ethanol are obtain the following results.

### **Fermentation**

Table 1 presents the results of the simulation of the fermentation stage.

Fermenter	Residence Time (H)	Volume (m <sup>3</sup> )	Heat Duty (kJ/s.)	Volumetric Water Flow (m <sup>3</sup> /h)
1	3.94	953,38	-7536,24	270,481
2	6.19	3112,15	-8779,01	316,330
3	13.82	30459,16	-10870,79	390,382
4	48.24	49273,93	-10039,89	300,145
Total	72.19	118792	-37225.9	1279,338

**Table 1** Fermentation Stage Results

Figure 5 shows the mass concentration profile in the fermenters simulated



Figure 5 Ethanol Concentration in the fermentation.

It is observed as the stoichiometry conversion of glucose is not proportional to production; this is due to the generation of unwanted products of the reactions (2) to (8) as methanol and acetic acid, among others. It was further noted that the train fermentation, the

concentration is increasing steadily, but the conversion of glucose is different for each reactor.

#### Ethanol Distillation

Figure 6 shows the profile results on the stripping column



**Figure 6** (a) Temperature profile in Stripping Column. (b) Concentration profile in the Vapor (Stripping)

The temperature increases linearly as it increases the number of stage, given that water has a higher boiling point that ethanol and thus the temperature will be higher where the concentration of water and organic compounds is higher. The gradient of ethanol concentration is higher in the steam in the area of the bottom of the column to the stage where remains constant until Stage 2, but more volatile compounds are enriching in the vapor upper zone of the column. The ethanol fumes out through the flow side, while leaving the volatile components for the distillate, which increases the mole fraction in this stream.



**Figure 7** (a) Temperature Profile in the Rectifier Column. (b) Concentration profile in the Vapor (Rectifier)

Figure 7 shows the profile results in rectifier column. The concentration of the less volatile components increase in the liquid, the temperature profile increases due to the concentration gradient components. The gradient of concentration of ethanol is higher in the zone below to the feed stage, due to temperature increase in stages near to the Reboiler. There is a change in the trend of the concentration of ethanol in the steam due to the feed stage. In the area above the stage feeding the driving force is much smaller because the ethanol is approaching its azeotropic point and is more difficult to separate the mixture.

Table 2 summarizes the results of the simulation of the ethanol distillation stage.

Parameters	Stripping Column (T-201)	Rectifier Column (T-202)	Recovery Column (T-203)
Condenser Duty	-493,285kJ/s	-39682,97 kJ/s.	-3710,52kJ/s.
Reboiler Duty		30330,31kJ/s.	3699,14kJ/s.
Steam Flow (45 psi)	2.27 kg /kg <sub>Et</sub>	1.55 kg/kg <sub>Et</sub>	0.19 kg/kg <sub>Et</sub>
Wt. % Ethanol Bottoms	0.05	0.03	0.03
Wt.% Ethanol Side Stream	48.1	0.78	
Wt.% Ethanol Distillate	70.2	0.951	0.95

**Table 2** Ethanol Distillation Results

## Ethanol Dehydration

Figure 8 shows the profile results on the column dehydration.

The ethanol concentration of through the stages of the column increases faster in the zone below to the feed stage, and then becomes constant because the few water that remains in the mixture. The temperature tends to decrease as the vapor flow is close to the column top, in the final stages there is a very high concentration end of heavy compounds (glycerol), representing a sharp rise in temperature . In the 50 stage show a temperature decrease because it corresponds to the feed stage. The temperature tends to decrease as the steam away from the stage of rehervidor, and in stage 2 reduces the temperature due to the condenser presence.

The glycerol of in the process, which complies the conditions for a good solvent because it is not evaporates and is removing water from the time they were fed, allows obtaining anhydrous ethanol, the less volatile compound (water) increases the concentration in the vapor in the section of depletion of the tower dehydration. In addition it appears that at the bottom of the column, the concentration of ethanol tends to zero, which suggests that the method is efficient.



**Figure 8** (a) Temperature Profile in the Dehydration Column. (b) Molar concentration profile on the liquid in dehydration column

Table 3 summarizes the results of the simulation of ethanol dehydration by extractive distillation

Parameters	Dehydration Column (T-301)	Regeneration Column (T-302)
Distillate Molar Flow	227.4 Kmol/h	98.6 Kmol/h
Condenser Duty	-3605,76 kJ/s	-552,83 kJ/s
Volumetric Water Flow	63,49 m <sup>3</sup> /h	8.79 m <sup>3</sup> /h
Reboiler Duty	4299,42 kJ/s	661,55 kJ/s
Vapor Flow (145 psig)	0.44 Kg/Kg <sub>Et</sub>	0.06 Kg/Kg <sub>Et</sub>
Wt.% Ethanol Bottoms	0.098	0.06
Wt.% Ethanol Distillate	99.99	6.9

 Table 3 Dehydration Results by Extractive Distillation

Table 4 summarizes the results of the simulation of ethanol dehydration by Adsorption with molecular sieves

**Table 4** Dehydration Results by Molecular Sieves

Parameter	Adsorber Bed	Desorber Bed
Electric Duty	18828 kW/h	1368000 kW/h
Wt.% Ethanol Output	99.99	49

## 4. Results Analysis

The highest energy consumption stage is the fermentation and here is where it is most needed water process, and the stage with greater use of steam is the stripping, because of the large amount of ethanol that is separated from the fluid fermented. Noting the trend can be said that energy consumption is decreasing as it moves through the process, namely the stage of fermentation is the process that consumes more energy and services, while dehydration is the stage where energy and services consumption is lower. The energy consumption and raw materials, varies in each of the simulations of the dehydration methods, which allows comparing the best suited to the Colombian industry, with the lowest operating cost and capital.

Table 5 shows the results of energy consumption in each of the simulations

Process Type	Energy Consumption (kJ/kg <sub>Et</sub> )	Steam Flow (kg/kg <sub>Et</sub> )	Volumetric Water Flow (m <sup>3</sup> /h)
Extractive Distillation (Glycerol)	38027.1	3.95 (45 psig) 0.5 (145 psig)	2850.6
Molecular Sieves	35557.8	4.01 (45 psig)	2778.32

 Table 5: Energy Consumption of each Simulation

Comparing energy consumption is concluded that the dehydration technology of adsorption with molecular sieves and extractive distillation with glycerol reported the lowest values, which makes them competitive and relevant to their study and implementation. The glycerol, due to increased production of biodiesel, the purchase price is low, which significantly reduces operating costs of extractive distillation.

Table 12 presents the initial investment costs for all three technologies. The initial investment costs are found to be high for molecular sieves, almost four times regarding the azeotropic distillation and twice regarding the extractive distillation. These high costs are justified by the level of automation required to control the cycles of adsorption/desorption beds to make a continuous operation. In most cases, the initial investment in a plant with

molecular sieves is 40% higher than a plant of equal capacity to use the distillation and quarrying (Gil, 2006).

Finally, the Extractive distillation constitutes a chance to study because it involves low energy consumption and industrial services moderate compared with other technologies. It is also important to note that investment costs are relatively high and not with the extractive distillation there is the option to make changes in the design of existing plants (revamping), with small capital investments to produce ethanol profitably in anhydrous.

Capacity	Extractive Distillation	Azeotropic Distillation	Molecular Sieves
300m <sup>3</sup> /day	USD\$650000	USD\$370000	US\$1170000
600m <sup>3</sup> /day	USD\$970000	USD\$600000	US\$1520000

### Table 12 Investment Cost

Source: (Gil, 2007)

# 5. Conclusions

The simulation allowed the identification technique dehydration alcohol by extractive distillation with Glycerol role as the best option to implement the production method to the reality of the Colombian industry.

Allowed to hear three variables, which are the most influential throughout the proceedings, which are:

- The pH of juice fermentation.
- The temperature reactors.
- The steam conditions injected into the stripping column.

Since any change in any of these variables affect the production of alcohol. It is important to mention that the above variables are not the only ones able to affect the process, since the pressure, the relationship between reflux in the columns, the ratio of solvent-feeding among others, can positively or negatively affect the process.

The current trend in the design and implementation process is one of the prerequisites energy efficiency of the processing operations and separation. The processes of ethanol dehydration not escape this trend and, hence, energy consumption defendant in the production of one kilogram of anhydrous ethanol is one of the main parameters in the application of technology. Apart from energy consumption, another important factor in selecting the best alternative technological ethanol dehydration is the consumption of industrial services required, as well as investment costs incurred during initial deployment of technology.

However, when taking into account the consumption of industrial services, is the extractive

distillation former glycerol excels at two other alternatives in terms of the required amounts of steam, water, electricity and agent of separation.

#### REFERENCES

- 1. Cardona, C.A., Sánchez, O.J. (2006). *Energy consumption analysis of integrated flowsheets for production of fuel ethanol from lignocellulosic biomass*, Energy No 31, pp. 2447-2459.
- 2. Cardona, C.A., Sánchez, O.J., Montoya, M.I, Quintero, J.A., *Simulación de los Procesos de Obtención de Etanol a partir de Caña de Azúcar y Maíz*, Scientia et Technica Año XI No 28 Octubre, pp. 187-192.
- 3. Carlson, E.C.,(1996). *Don't Gamble With Physical Properties for Simulations*, Chemical Engineering Process, Octubre de 1996, pp. 35-46.
- 4. Fogler, H.S., (2001). *Elementos de Ingeniería de las Reacciones Químicas*. Ed. Prentice-Hall, Capitulo 4, Capitulo 5.
- 5. Gil, I.D., (2006), *Diseño, montaje y puesta en marcha de una destilación extractiva para la producción de alcohol anhidro*. Tesis para obtener el título de Magister en Ingeniería Química, Universidad Nacional de Colombia.
- Gil, I.D., Aguilar, J., Rodríguez, G., Caicedo, L.A., Uyazán, A.M. (2006), *Producción de Alcohol Carburante por Destilación Extractiva: Simulación del proceso con Glicerol.* Ingeniería e Investigación, abril, año/ Vol.26, numero 001, pp. 45-50.
- 7. Grisales, P.A., Ríos, L.A., Triana M. *Diseño de un proceso de producción de etanol anhidro a partir de jugo de caña*. Escuela de Ingeniería Química, Universidad del Valle
- 8. Honorato, Flavio., Rodrigues, Maria., Maugery Francisco., (1999). *Dynamic modelling, simulation and optimization of an extractive continuous alcoholic fermentation process*. Journal of Chemical Technology and Biotechnology No 74, pp. 176-182.
- 9. Jacques, K., Lyons, T.P., Kelsall, D.R., (1999). *The Alcohol Text Book*. Ed. Nottingham University Press, 1999, Chapter 5, Chapter 9, Chapter 16, Chapter 17, Chapter 18.
- 10. Kister, H., (1990). *Distillation Operation*. Ed. McGraw-hill, 1990, Chapter 2, chapter 4.
- 11. Seider, D.W., Seader, J.D., Lewin, L.W.(2003). *Product and Process Design Principles.* Ed. John Wiley & Sons, Chapter 3, Chapter 4.