

VOL. 35, 2013



DOI: 10.3303/CET1335087

Guest Editors: Petar Varbanov, Jiří Klemeš, Panos Seferlis, Athanasios I. Papadopoulos, Spyros Voutetakis Copyright © 2013, AIDIC Servizi S.r.l., ISBN 978-88-95608-26-6; ISSN 1974-9791

Thermo-Economic Optimization of Integrated First and Second Generation Sugarcane Ethanol Plant

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The sugarcane industry has been responsible in some countries for the production of most of the sugar and ethanol available in the world for internal and external markets. In this sector, ethanol can be produced by fermentation of sugars obtained directly from sugarcane biomass, commonly called 1st generation ethanol. New processes using the enzymatic hydrolysis technology of lignocellulosic residues like bagasse and sugarcane leaves as feedstock can increase the ethanol production in these plants, reducing the land requirements and the environmental of impact biofuels production in large scale. The lignocellulosic ethanol production using enzymatic hydrolysis technology is one of the most promising alternatives of 2nd generation biofuels, due to its high conversion efficiencies and low environment impact. Some problems like high water consumption and enzymes costs must be overcome in order to reach commercial scale. The process integration and thermo-economic optimization of the process can be important for the design of this process in a sugarcane autonomous distillery aiming at the cost and environmental impact reduction. In this paper a process integration of the sugarcane ethanol distillery model is carried out taking into account 1st and 2nd generation processes in the same site using sugars and bagasse as feedstock respectively. Conflictive objectives such as maximization of the electricity or ethanol production are adopted in a multi-objective optimization technique using evolutionary algorithms, in order to provide a set of candidate solutions considering different configurations of the ethanol production process design.

1. Introduction

The conversion of biomass into biofuels represents an important option for both the exploitation of an alternative source of energy and the reduction of polluting gases, mainly carbon dioxide (Cardona-Alzate and Sanchez-Toro, 2006).

Ethanol produced from lignocellulosic biomass is examined as a large scale transportation fuel. Desirable features include fuel properties of ethanol as well as benefits with respect to urban air quality, global climate change, balance of trade, and energy security. Energy balance, feed-stock supply, and environmental impact considerations are not seen as significant barriers to the widespread use of fuel ethanol derived from lignocellulosic biomass, being the conversion economics a key obstacle to be overcome (Dias et al., 2012).

The conversion process from lignocellulosic biomass to ethanol consists basically of four steps: pretreatment, enzymatic hydrolysis, fermentation, and distillation. Pre-treatment is a necessary step to facilitate the enzymatic attack of lignocellulosic residues. Steam explosion is recognized as an efficient pre-treatment method where the raw material is exposed to pressurized steam followed by rapid reduction in pressure resulting in substantial breakdown of the lignocellulosic structure, hydrolysis of the hemicellulose fraction, depolymerization of the lignin components and defibration. Therefore, the accessibility of the cellulose components to degradation by enzymes is greatly increased (Cara et al., 2008).

Please cite this article as: Ensinas A.V., Codina V., Marechal F., Albarelli J., Silva M.A., 2013, Thermo-economic optimization of integrated first and second generation sugarcane ethanol plant, Chemical Engineering Transactions, 35, 523-528 DOI:10.3303/CET1335087

2. Process Description

The simulation of the whole process using a flowsheeting software is carried considering technology available in modern ethanol distilleries in Brazil, including sugarcane dry cleaning, concentration in multieffect evaporators, sterilization of the juice before entering the fermentation system and ethanol dehydration using Monoethylene Glycol (MEG).

2.1 First generation ethanol

The 1st generation ethanol distilleries is modelled considering the average sugarcane composition reported by Dias et al. (2009) in mass basis: 13.3 % sucrose, 4.77 cellulose, 4.53 % hemicellulose, 2.62 % lignin, 0.62 % reduced sugars, 0.20 minerals, 1.79 % impurities, 0.60 % soil and 71.57 % of water. The following steps are considered in the process design.

Juice extraction and treatment

The sugarcane is processed following current technology available in ethanol distilleries with dry cleaning system using air-blowers to remove soil and other big size particles that can affect negatively the industrial process. After that, a crushing system is used to separate fiber and sugarcane juice using knives, shredders and milling tandems. Water is added to improve the extraction of the juice, that can leave this system with 12-14°Brix depending of the operation and the system design. The bagasse is separated from the liquid stream with a moisture content of 50wt% and is composed mainly by cellulose, hemicellulose, lignin and ash(Palacios-Bereche et al. 2011).

The juice is treated before concentration in order to remove impurities and improve the fermentation step. Some chemicals like phosphoric acid and CaOH are used to improve the process and units of heating, decantation and filtration are commonly used.

Concentration and sterilization

In order to increase the concentration of the must for the fermentation process part of the treated juice is concentrated until 65° Brix in multi-effect evaporators and after that it is mixed with the rest of the by-passed juice, obtaining a glucose content of 20 % for the conversion into ethanol.

The sterilization is done using a treatment type HTST (High Temperature Short Time). In this treatment the must is heated until 130 °C, staying at this temperature for approximately 30 min. After that there is a fast cooling until fermentation temperature in the range of 32 °C (Dias et al. 2009).

This treatment is done in order to reduce contamination by microorganism that could affect the fermentation process in a negative way.

Fermentation

In industrial fermentation, sugarcane juice is used as a source of sugars for the production of ethanol. Sucrose, the most abundant sugar, is hydrolyzed into glucose and fructose, which are converted into ethanol and carbon dioxide, in reactions catalyzed by the yeast *Saccharomyces cerevisiae* (Mariano et al. 2013).

Fermentation process was simulated considering a stoichiometric reactor, with all the sucrose converted in glucose in a first reaction and the conversion of glucose into ethanol and CO₂ with a yield of 89 %. By-products formation includes succinic acid, acetic acid and glycerol according to (Dias et al., 2011).

Nowadays, in Brazilian sugarcane industry the most common technology for ethanol production is Batch fed fermentation with recycle of cells (*Melle Boinot* process).

This process formerly introduced by French distilleries to Brazil in 30's to ferment molasses has been improved to work on a large scale of must composed by a mixture of cane juice, syrups and rich molasses. The process is a batch fed fermentation with cell recycle. At the end of the fermentation the wine is centrifuged to recover most of the yeast, which is submitted to an acid treatment diluting the cream with water and dropping the pH with sulphuric acid.

Some reactions occur such as the killing of bacteria and harmful yeasts, and the reduction of intracellular activity of ethanol. The aeration of the fermenter restores the activity of yeasts. Once ready, this inoculum is sent to fermentation vats, where alcoholic fermentation starts again (Dias et al., 2012).

Distillation

The wine produced in fermentation process goes to distillation unit where hydrated fuel ethanol is produced with ethanol concentration between 92.6 and 93.8 wt% (Ensinas et al. 2007).

The most common configuration of ethanol distillation, in Brazilian distilleries, uses 5 columns: A, A1, D, B and B1. The column A is known as wine stripping column of wine. The column A1 is the wine rectification column. The column D is for concentration of second grade alcohol. The joint of these three columns is

called as distillation column. The column B is the rectification column and the column B1 is the stripping column. This joint is called as rectification column where hydrated fuel ethanol is obtained.

Extractive distillation with MEG is considered as dehydration technology. Two columns are modelled: the extractive and the recuperation columns . The first column receives the hydrated ethanol in vapour phase, coming to distillation process near to the bottom and the solvent MEG near to the top. As product there is, in the top, the anhydrous fuel ethanol AEHC, while in the bottom the stream composed by a mixture of solvent and water, which goes to recuperation column. In the recuperation column water is obtained at the top while recuperated MEG is obtained at the bottom. This column has approximately 10 stages and operates at pressure of 20 kPa in order to get moderate temperatures in the range of 150 °C at the bottom column avoiding in this way the solvent decomposition.

2.2 Second generation ethanol

A number of different processes have long been envisioned to produce second-generation ethanol. The SO₂-catalyzed steam pre-treatment followed by enzymatic hydrolysis is a promising alternative that has been studied by many different research groups. Steam explosion pre-treatment renders biomass more readily digestible by enzymes requiring little or no chemical input and thus being more environmental friendly relative to other technologies. The SO₂-catalyzed steam pre-treatment followed by enzymatic hydrolysis process for bagasse is studied in this paper. Data was gathered from the best condition studied for this process by (Carrasco et al., 2010).

The degradation of the lignocellulosic materials requires two steps; the first step is the pre-treatment for the solubilisation of the hemicelluloses and releasing the lignin and second step is the hydrolysis of cellulose.

The purpose of the pre-treatment is to remove lignin and hemicelluloses, reduce cellulose crystallinity, and increase the porosity and contact area of the materials to let the cellulase enzymes gain access to the cellulose molecules. During the pre-treatment of lignocellulosic material the hemicelluloses fraction is also hydrolyzed.

In a step before the pre-treatment with steam explosion technology, addition of SO_2 is considered a washing step of bagasse in order to reduce amounts of ashes and impurities. This previous washing of bagasse has the advantage of using fewer amounts of reactants in posterior steps of the process.

For the simulation of the pre-treatment reactor it is considered the formation of xylose and acetic acid from hemicelluloses, the formation of furfural from xylose and the formation of glucose from cellulose.

Product yields for pre-treatment reactor (xylose 61.4 %, acetic acid 9.2 %, glucose 4.1 % and furfural 5.1 %) were calculated using data from Carrasco et al. (2010). After pre-treatment the pulp pre-treated is washed in order to release xyloses and lignin which highly affect the enzymatic hydrolysis.

The hydrolysis step takes place in several reactors at 50 °C and residence time of 24 h and is done using cellulase concentration of 15 FPU/g of biomass (enzyme activity 65 FPU/g) and β -glucosidase concentration of 0.9 IU/g of biomass (17 IU of enzyme activity/g) (Carrasco et al., 2010). Cellulose and hemicellulose conversion are 69.2 % and 35.7 % respectively.

The integration of 1st and 2nd generation plants occurs using the same fermentation system for the sugarcane juice and the hydrolysis liquor. The ethanol process was completed with the same distillation and dehydration steps used in the 1st generation plant. For the integration of hydrolysis process to traditional plants of ethanol, the liquor glucose liquor is concentrated up to 20 % in a multi-effect evaporation system in order to be mixed with the must of sugarcane juice (Figure 1).

3. Methodology

A flowsheeting model of the process is developed in the ASPEN PLUS software in order to compute the mass and energy balance of the 1st and 2nd generation ethanol plants. A thermo-economic model of the production process is solved in MATLAB based platform (OSMOSE) using state variables obtained in the detailed simulation of all the equipment and conversion steps of the process.



Figure 1: Flowsheet for the 1st and 2nd generation ethanol production

After that the optimization problem is solved with the decomposition method, divided in two parts: a master and a slave optimization. The energy-integration model is sent to the slave optimisation which runs a combined mass and energy integration in order to reduce the operating cost of the system, using a Mixed Integer Linear Programming solver. Subsequent, the master problem, subject to the results of the slave sub-problem, deals with the units sizing and internal model variables and it is solved as multi-objective optimization with conflictive objective such as maximization of electricity or ethanol production. As shown in Figure 2, the master problem is solved using an evolutionary multi-objective optimizer.



Figure 2: Design methodology: thermo economic optimisation

The exergy efficiency (η) and the yearly total cost (C_t) are two of the performance indicators in the study used for comparing the different alternatives.

$$\eta = \frac{\sum \Delta k_{ethanol}^{o} \vec{m}_{ethanol}^{+} \dot{E}^{-}}{\Delta k_{sugarcane}^{o} \vec{m}_{sugarcane}^{+} + \Delta k_{leaves}^{o} \vec{m}_{leaves}^{+} + \dot{E}^{+}}$$
(1)

(2)

$$C_t = C_{inv} + C_{enz} + C_{sugarcane} + C_{elec} + C_{leaves}$$

In Eq.(1), Δk^o is the exergy value of a material stream and \dot{m} is the mass flow rate for that stream. \dot{E}^- represents the net electricity produced by the plant and \dot{E}^+ and the electricity imported from the grid when the net balance is negative. In Eq.(2), the yearly total cost is calculated considering annualized investment (C_{inv}) and the operating expenses like the enzymes cost (C_{enz}), sugar cane cost ($C_{sugarcane}$), electricity imported or exported (C_{elec}) and leaves cost (C_{leaves}). Detailed estimation of investment for each piece of equipment is calculated with the method available in Ulrich (2004), according to the size, retention time and other characteristics defined in the physical model. Table 1 sums up the parameters that are used for computing these indicators.

4. Results

A multi-objective optimisation has been done, setting the electricity production (kWh/t_{cane}) and the produced ethanol (L/t_{cane}) as objective functions to be maximized. The decision variables for the optimization are the percentage of bagasse for 2^{nd} generation ethanol production and the glucose concentration between each step of the multi-effect evaporation system. Setting the concentration as

decision variable allows to improve the integration between the vapour bleeding and the rest of the process.

M&S Index	1597.7	$\Delta k_{sugarcane}^{o}$ ¹ (wet base)	4.52 MJ/kg	Ethanol price	0.72 US\$/L
Interest rate	10 %	$\Delta k_{leaves}^{o^{-1}}$ (wet base)	15.97 MJ/kg	Enzymes price ²	1250 US\$/t
Life time	25 y	Imported electricity price ¹	70.51 US\$/MWh	Sugar cane ²	31.17 US\$/t
Working days	200	Exported electricity price ¹	51.00 US\$/MWh	Leaves price ²	15.02 US\$/t
$\Delta k_{ethanol}^{o}$ 1	27.15 MJ/kg				
¹ (Oieda et al. 2011): ² (Albarelli 2013)				

Table 1: Parameters for the exergy efficiency and the economic evaluation

al. 2011); ²(Albarelli 2013)

Figures 3 and 4 are the composites for two systems configuration, with 16% and 75% of the bagasse for the second generation respectively. The lower is the quantity of bagasse used for 2nd G ethanol, the higher is the amount of electricity produced by the cogeneration system as the heat demand decreases and there is more bagasse available for the burner.



Figure 5 represents the Pareto front for the two objective defined in the multi-optimization problem. The increase in the ethanol production is due to the higher quantity of bagasse sent to the 2nd generation process.



Figure 5: Electricity-ethanol production Pareto

Figure 6: Benefit and cost for the ethanol production

Enzymes cost, net electricity produced and capital annualized investment can affect the benefit significantly and can be seen in the Figure 6. By comparing the slopes for the ethanol benefit and the enzymes expenses, it can be stated that there is a direct impact of the enzymes expenses in the ethanol production cost. The production cost for the 1st generation ethanol is calculated as 0.49 US\$/L, while the marginal for the 2nd generation ethanol is within the interval 2-2.6 US\$/L, which is derived from the Eq.(3).

 $P_{2G} = \frac{F_{1G+2G} \cdot P_{1G+2G} - F_{1G} \cdot P_{1G}}{F_{1G+2G} - F_{1G}}$

where *P* denotes the ethanol total cost and F the amount of ethanol produced from juice (1G) or juice and bagasse (1G + 2G). P_{2G} increases when more bagasse is used for the 2nd generation as the electricity production decreases.

The pareto front (Figure 5) and the electricity cost curve (Figure 6) present a change in the trend due to the energy integration problem solved at the slave optimization level. Figure 6 shows that when more than 72% (91.3 L/t cane) of the bagasse is sent to the 2^{nd} generation process, the electricity production of the cogeneration system is lower than the demand so it is necessary to import electricity from the grid.

The η of the system is between 39-41 % from 10 to 50 % of bagasse for the 2ndgeneration plant, decreasing for higher values. After 50 %, η is strongly affected by the reduction of the electricity production in the cogeneration system, dropping to 34.5 % for 85 % of bagasse 2ndG.

5. Conclusions

The main problem of the 2^{nd} generation ethanol is the high cost of the enzymes. It can be stated that even having an ideal integration for the 2^{nd} generation process, it will not be profitable unless a high decrease in the enzymes price happens. It worth to say that in this study has been taken an enzyme cost of 1,250 \$/t, which is a value for a future scenario where the cost of the enzymes is expected to be more competitive. Due to the high cost and low exergetic efficiency of the 2^{nd} generation process, other kind of technologies for bagasse valorisation should be studied, as for example the production of highly added value products for the chemical industry. The production of ethanol from xylose would be another possibility for increasing the process profitability but the fermentation of the C5 sugars is still under development.

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