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MULTI-OBJECTIVE OPTIMIZATION OF AN INDUSTRIAL PROCESS OF BIOMASS CONVERSION INTO ENERGY VECTORS: SUGARCANE TO ETHANOL AND ELECTRICITY

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Abstract. *The main objective of this work is to investigate the impacts of integrating new biomass deconstruction technologies into an existing agro-industrial production process in terms of its new multi-objective optimal operating conditions. A comprehensive model describing unit operations and chemical reactions is simulated by the Monte Carlo method. The results reveal that the input variables have specific characteristics when the corresponding operating states lay near the maximum energy limit (Pareto frontier). Optimal ethanol and electricity generation probability density functions show that optimality is more likely to be achieved at low burning bagasse rates, due to high energy demands of the dewatering operation. Also, choosing the pretreatment/fermentation pathway for hemicelluloses increases the probability of optimum operation and adds robustness to the process in the sense that optimality is less sensitive to fiber composition and humidity. This is so because of hemicelluloses' relatively low energy content in contrast with good yield/fermentation characteristics. Finally, if hemicelluloses are should be burned, it is better to have feedstocks richer in lignin because of its higher energy content. These are extremely rich and useful information, not only to the more immediate decisions regarding the industrial conversion, but also to agricultural production issues and feedstock logistics.*

Keywords: *industrial biomass processing; multi-objective optimization; biofuels; bioenergy; efficiency; biorefinery*

Introduction

Ethanol used in flex-fuel cars or simply as an additive for gasoline constitutes one of the most promising possibilities of displacing fossil fuel resources. It is thus expected a great increase in international demand for this product and, in fact, several countries passed bills mandating an increasing production and consumption of ethanol for transportation fuel. The 2nd generation biofuels produced from ligno-cellulosic fibers, a major and universal component in plant cells walls constitutes an attractive and promising alternative to increase ethanol production and to produce energy. For instance, a maize producer can sell grains to an animal feed industry and use leafs, stalk, and cobs to produce cellulosic ethanol. A great variety of agricultural feedstock could also be used to produce it, such as sugarcane bagasse, miscanthus, switchgrass, eucalyptus etc., as well as many types of industrial wastes such as saw-dust, textile, paper, cardboard remains, etc.

In fact, biomass has become an important alternative feedstock for energy production and carbon based chemicals. Recent reports reveal that global biomass technical potentials could supply as much as four times the current global needs. Although the assumptions behind these calculations lead to over estimated numbers, because they ignore all competing land uses and socioeconomic constraints (Slade, *et al.*,2011 and Leite, *et al.*, 2009a), these results give a real perspective of the important role that biomass can play is displacing fossil resources. The biorefinery concept emerged as new agro-industrial paradigm in which biomass is carefully deconstructed to produce low-value/large-volume liquid transportation fuel such as biodiesel or bioethanol and, additionally, to produce low-volume/high-value products such as pharmaceuticals and nutritional compounds. It is just realistic to suppose that many of these new biorefineries will evolve from the existing biomass processing industries. This actually constitutes the central objective of this work: to investigate and quantify the impact of integrating new biomass deconstruction technologies into an existing agro-industrial production model in terms of its new multi-objective optimal operating conditions. Although we will base this work on the Brazilian sugarcane sector, the same approach is applicable to other agricultural crops.

1. THE REFERENCE SUGARCANE PROCESSING PLANT WITH INTEGRATED PRODUCTION OF 2G ETHANOL

The average sugarcane productivity in the state of São Paulo, Brazil, is of 85 tsc/ha. Thus, adopting a harvesting period of 210 days, the resulting round-the-clock biomass processing flux will be about 500 tsc/h. The equipment necessary to process this biomass flux, according to the operations described above, will be able to produce approximately 65 t/h of refined sugar or 43 m^3/h of hydrous ethanol during the harvesting period. In the process, after

tsc = tonnes of sugarcane
ha = hectare
t = tonne

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separation of straw and extraction of sucrose, 150 t/h of bagasse will be generated (80% moisture content) which, after being dewatered to reduce moisture content to 50%, can produce electricity at the rate of 50 MW, although this number can vary significantly depending on fiber content, boiler pressure, etc. More specifically, bioelectricity generation is based on cogeneration steam cycles at pressures around 2.2 MPa, from which it is possible to attend internal energy demands and still produce small amounts of bagasse (5–10% of biomass) and electricity surpluses (0–10kWh/tsc).

Recently, more elaborated engineering design techniques, new materials and more skilled fabrication technology enabled the development of more efficient and better integrated processes equipped with high-pressure steam systems (e.g. 6.5 MPa @ 480^{o}C; some units with 12.0 MPa @ 540^{o}C) capable of generating over 100 kWh/tsc (Seabra and Macedo, 2011). Residues are also generated in the process, the most important ones being 1 t/h of filter cake from filtration of sugarcane juice, 2 t/h of CO_2 from fermentation and 500 m^3/h of vinasse.

Production of second generation (2G) ethanol should be integrated into this existing industrial model. The use of ligno-cellulosic biomasses for ethanol production can only occur if its recalcitrance is broken, that is, if its sugar monomers have been previously made available for the fermentation process. This is better done in a two stages process: 1) dismantling of ligno-cellulosic macro-structures (pretreatment) and, subsequently, 2) rupture of glycosidic bonds (hydrolysis). Several pretreatment techniques have been developed, particularly for materials such as wheat straw, corncobs, and various grasses. Traditional techniques include acid treatment and steam explosion with or without ammonia or organic solvents.

2. ENERGY ANALYSIS OF THE INTEGRATED 1G/2G/ELECTRICITY PRODUCTION MODEL

The energy content of sugarcane is distributed by juice, straw and bagasse, approximately in equal proportions. The diagram in Fig. 1 shows the stages of mechanical and extraction processing for separating these three components which subsequently follow different process for conversion to ethanol (fermentation and juice distillation) and electricity (production of steam by burning bagasse and straw). After the pre-treatment and hydrolysis processes, the fermentable sugars can be fermented together with the juice and increase the production of ethanol. The lignin is non-fermentable and it is also liberated in this process. Due to its high heating value, lignin can be used to offset the energy deficit by reducing the amount of burnt bagasse, creating a degree of freedom related to bagasse fractions destined for burning and cellulosic ethanol production. The integrated production of electricity and first and second generation ethanol is illustrated in Fig. 1. An energetic analysis of this model will be made with a description of the thermodynamic cycle of conversion and constituent fractions of bagasse fiber, as well as by function of quantities of fiber constituents burned and converted into ethanol.

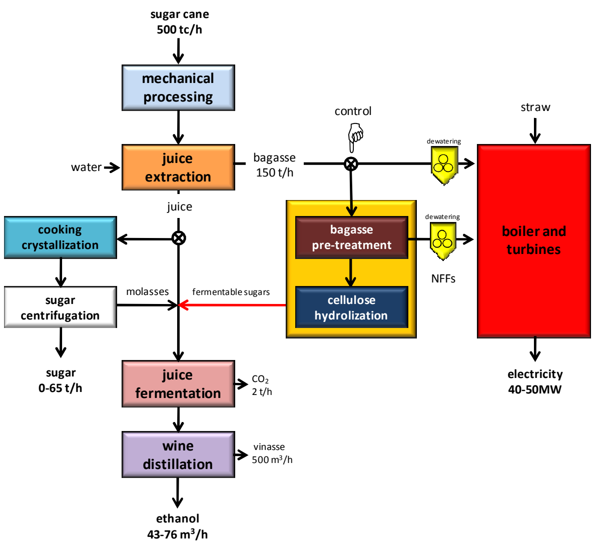

Figure 1. Reference sugarcane industrial processing model

The main question in the optimization is the ideal "tune" of the process as a whole, refers to different energy demands associated with the units of operations for each route of conversion. For example, it is known that the drying water process consumes large amounts of energy and its efficiency falls with the rate of processing, requiring more energy so as not to degrade its performance. Therefore, reducing the quantity of burnt bagasse will significantly decrease the energy demand in a first analysis. However, the efficiency of combustion tends to be greater for a bigger boiler, an effect which can cancel the gain in the drying water operation. Thus, the optimization problem consists in setting the control variable in order maximize ethanol production and electricity generation, i.e. two simultaneous

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objectives, given all possible random variations of other intervening variables, such as fiber constitution, bagasse humidity, etc. This model will be described in detail below and it is described in Fig. 2.

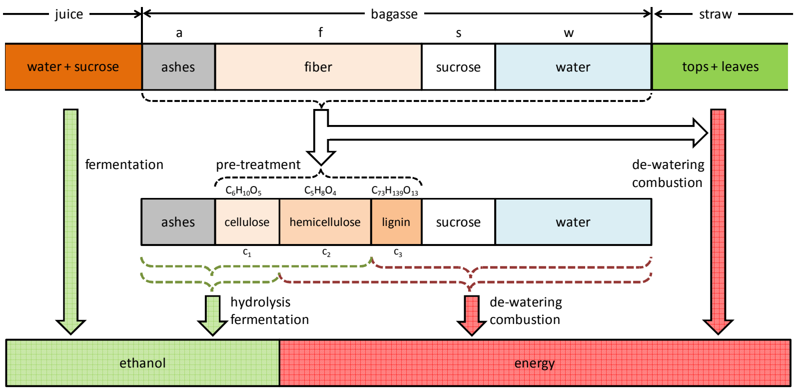

Figure 2. Sugarcane constituents conversion pathways (hemicelluloses are burned or fermented)

2.1 HYDROTHERMAL PRETREATMENT

Ideal pre-treatment should produce cellulose and hemicelluloses highly available to hydrolysation, yield non-degenerated pentoses and hexoses, enhance lignin separation, avoid the formation of inhibitory agents, needless of additional mechanical processing and should be possible to implement on simple equipment, made with low cost material, such as: 1) a progressive cavity pump to elevate the pressure and inject a mixture of water and biomass into a 2) large volume exchanger, to provide heat and ensure necessary residence time at pretreatment conditions, followed by 3) an expansion valve to impose an explosive depressurization and 4) a cyclone separator to separate gaseous fractions from liquid-solid fractions, as shown in Fig. 3.

Cellulose and hemicelluloses become highly available to hydrolysis even under mild conditions which, consequently, increases production rates with minimum degradation of component sugars.

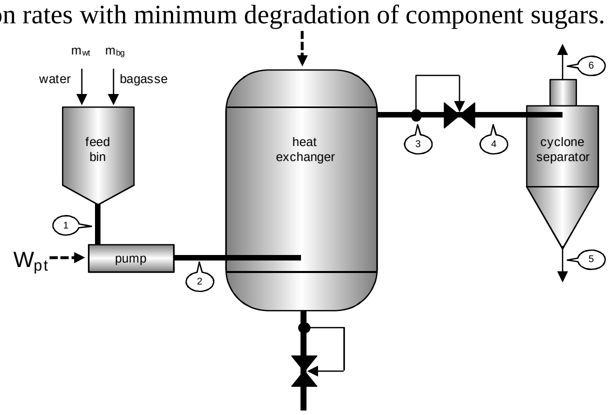

Figure 3. Hydrothermal pretreatment processes and equipments

The energy necessary to perform these operations can be estimated by analyzing the thermodynamic transformations experienced by water.

2.2 REACTION YIELDS AND EFFICIENCIES

Sugarcane bagasse is basically composed of ligno-cellulosic fibers, water (humidity), residual sucrose or other extractives and ashes. Ashes are commonly associated with gravel and dirt collected by mechanical harvesting machines. Typical fiber contents vary between 40-50% while ashes and residual sucrose are within 0-4%. Humidity values depend on processing conditions and after dewatering may vary between 45-60% (Leite, *et al.*, 2009a). Fibers are predominantly composed of lignin, cellulose and hemicelluloses. Lignin is usually employed in power generation because it has high energy content and it is not efficiently fermented. The net amounts of cellulose and hemicelluloses obtained from pre-treated fibers are usually expressed in terms of percentage yields based on the initial masses of ligno-

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cellulosic feedstock. Typical values obtained from literature are listed in Tab. 1, including the ones adopted in this work.

Table 1. Sugarcane fiber composition and pretreatment yields

fiber composition (db)					
	Furlan, *et al.*,2012	Hamelinck, 2005	Wolf, 2011	Toor, 2011	Figuerut, 2006
cellulose	39	40 - 60	38.8+1.4	39	32 - 48
hemicelluloses	37	20 - 40	29.4+1.7	24.9	27 - 32
lignin	21	10 - 25	21.7+0.7	23.1	19 - 24

The enzymatic hydrolysis process consists in converting cellulose and hemicelluloses into fermentable sugars, catalyzed by enzyme cocktails. Cellulose hydrolysis into glucose is given by the net equation $[C_6H_{10}O_5]_n + nH_2O \rightarrow nC_6H_{12}O_6$, from which it is possible to write the following equation relating both mass flow rates:

$$\dot{m}_{gluc} = \eta_{gluc} \cdot \frac{180.01}{162.14} \cdot \dot{m}_{cel} \quad (1)$$

where η_{gluc} quantifies the efficiency of the reaction. Subsequent fermentation of glucose into ethanol occurs according with the net equation $C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$. The corresponding mass balance equation is given by

$$\dot{m}_{geth} = \eta_{geth} \cdot \frac{2}{1} \cdot \frac{46.07}{180.17} \dot{m}_{gluc} \quad (2)$$

in which η_{geth} represents the ethanol to glucose conversion efficiency. These equations can be combined to calculate the mass flow rate of 2G ethanol produced from a given mass flow rate of cellulose.

Hemicelluloses are branched heteropolymers containing xylan, glucuronoxylan, arabinoxylan, glucomannan, and xyloglucan in different proportions. Sugarcane bagasse hydrolysis of these molecules produces predominantly xylose according with the net equation $[C_5H_8O_4]_n + nH_2O \rightarrow nC_5H_{10}O_5$, whose fermentation is given by $3C_5H_{10}O_5 \rightarrow 5C_2H_5OH + 5CO_2$. Denoting the associated efficiencies by η_{xylo} and η_{xeth}, the corresponding mass balance equations are

$$\dot{m}_{xylo} = \eta_{xylo} \cdot \frac{2}{1} \cdot \frac{150.12}{132.11} \dot{m}_{hem} \quad (3)$$

$$\dot{m}_{xeth} = \eta_{xeth} \cdot \frac{5}{3} \cdot \frac{46.07}{150.13} \dot{m}_{xylo} \quad (4)$$

Analogously to cellulose, the mass flow rate of hemicelluloses obtained from the pretreatment process can be fed into these equations to calculate how much ethanol is produced by fermenting xylose.

The importance of introducing the efficiencies in the above equations is that, in fact, they represent simplified versions of the multiple and interdependent chemical reactions that take place, both in hydrolysis and fermentation. Thus, the generation of byproducts and other process complexities that lead to losses and that are not being considered at first can be accounted for through these reaction efficiencies. Typical values reported in open scientific literature are listed in Tab. 2.

Table 2. Reaction efficiencies in equations (1) to (4)

reaction	reaction efficiency (%)				
	symbol	Furlan, *et al.*,2012	Wolf, 2011	Hamelinck, 2005	Seabra, 2008
cellulose $\rightarrow$ glucose	η_{gluc}	80		75-85	95
glucose $\rightarrow$ ethanol	η_{geth}	90		90-95	95
hemicellulose $\rightarrow$ xylose	η_{xylo}	20.4	67.8	88-98	48
xylose $\rightarrow$ ethanol	η_{xeth}	65		80-90	85

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2.3 BAGASSE DEWATERING

Bagasse dewatering is a crucial operation for an efficient and safe combustion process. Safety issues arise because combustion of high humidity solid fuels is problematic, particularly due to its tendency to aggregate, what increases the possibility of explosion. After sucrose extraction, bagasse humidity is approximately 80% with a residual sucrose content of less than 2%. One or two additional roll mills are used to reduce humidity to approximately 50-55%, which is the usual specified maximum biomass humidity for an industrial water tube boiler. The extracted water is usually recirculated through the extraction system to improve residual sucrose retrieval.

The dewatering mills can be controlled by adjusting the processing speed and hydraulic load in order to maintain humidity as close as possible to the set point, usually around 50%. Thus, Hugot's equation (Hugot, 1969) and what is known about the governing physical phenomena permit to propose a simplified model for assessing the driving power. Considering that the processing rate is proportional to the product of $\omega \cdot D/2$ because

$$\dot{m}_{bg} = \rho_{bg} e_p \; LV_{bg} = \rho_{bg} e_p \; Lr \frac{\omega D}{2} \qquad (5)$$

we will adopt the following simplified model

$$W_{pr} = K \cdot \left(\frac{\dot{m}_{bg}}{\dot{m}_{nom}}\right)^{1+a} \qquad (6)$$

where $\dot{m}_{nom}$ is the nominal mass processing rate and k and a are adjusted empirically. Using data provided by different manufacturers of similar dewatering mills we obtained K = 2.91 MW and a = 0.0136 for m_{non} = 160 t/h, which is consistent with the usual values of 15-25 kWh per tonne of bagasse found in practice (Van Breda, 1984 and Wienese, 1987). Considering our reference sugarcane processing plant, dewatering power demand is about 2.73 MW to process its 150 t/h of bagasse, what shows that dewatering trough mechanical devices is effectively a very energy intensive operation.

2.4 BIOMASS COMBUSTION AND POWER GENERATION

The maximum amount of heat released by bagasse combustion depends on the lower heating values of its energy constituents whose combustion equations are given by:

sucrose: $C_{12}H_{22}O_{11} + 12\,(O_2 + 3.76\,N_2) \rightarrow 12\,CO_2 + 11\,H_2O + 45.12\,N_2$ (7)

cellulose: $C_6H_{10}O_5 + 4.5\,(O_2 + 3.76\,N_2) \rightarrow 6\,CO_2 + 5\,H_2O + 16.92\,N_2$ (8)

hemicellulose: $C_5H_8O_4 + 5\,(O_2 + 3.76\,N_2) \rightarrow 5\,CO_2 + 4\,H_2O + 18.80\,N_2$ (9)

lignin: $C_{73}H_{139}O_{13} + 101.25\,(O_2 + 3.76\,N_2) \rightarrow 73\,CO_2 + 69.5\,H_2O + 190.35\,N_2$ (10)

The individual higher heating values (HHV) can be calculated from the fuel elemental composition according with Friedl, *et al*., 2005.

$$HHV(C, H, N) = 3.55C^2 - 232C - 223OH + 51.22CH + 131N + 20600 \qquad (11)$$

where *HHV* is in kJ/kg and *C*, *H* and *N* represent carbon, hydrogen and nitrogen mass percentage composition of the fuel. Considering that varying percentages of residual sucrose, cellulose, hemicelluloses and lignin constitute the bagasse to be burned, the resulting higher heating value is calculated according with the following formula:

$$HHV_{bagasse} = \frac{f}{\sum c_k} \cdot \textstyle\sum_k c_k . HHV_k + s . HHV_{sucrose} \qquad (12)$$

where *f* and *s* denote respectively the fiber and residual sucrose contents. Likewise, HHV_k and c_k are, respectively, the higher heating value and proportion of the k-th fiber constituent, given in Tab. 3. The lower heating value is calculated by subtracting the energy necessary to vaporize water formed during combustion as well as remaining from the dewatering process. This can be calculated from the bagasse hydrogen elemental percentage (H) given by:

$$H_{bagasse} = \frac{f}{\sum c_k} . \sum_k c_k . H_k + s . H_{sucrose} \tag{13}$$

The lower heating values (LHV) are then calculates by the formula:

$$LHV = (1 - w) \left[HHV - \lambda . \left(\frac{w}{1 - w} + 0.09H \right) \right] \tag{14}$$

where λ is the latent heat of water (2.31 MJ/kg @ 25°C). Nitrogen oxidation and heat absorption can be neglected.

Table 3. Bagasse constituents' elemental compositions and corresponding higher and lower heating values

Bagasse/fiber Component	**Average Formula**	**Percent mass composition**			**HHV (MJ/kg) (w=0%)**	**LHV (MJ/kg) (w=50%)**
		C	**H**	**O**		
Sucrose	$C_{12}H_{22}O_{11}$	42.10	6.48	51.42	16.64	6.49
Cellulose	$C_6H_{10}O_5$	44.44	6.21	49.34	17.58	6.99
Hemicellulose	$C_5H_8O_4$	45.45	6.10	48.44	17.98	7.20
Lignin	$C_{73}H_{139}O_{13}$	71.58	11.44	16.98	38.60	16.96

As depicted in Fig. 2, non-fermentable fractions (NFFs) of the pre-treated bagasse are used to increase electricity generation. The net amount of heat produced by burning these NFFs depends on the resulting lower heating values which can be determined following the same procedure described above. Additional assumptions are the following: 1) NFFs are composed of lignin in one case and lignin+ hemicelluloses in the other case, at the same original proportions, 2) residual sucrose is still present in NFFs due to its solubility in water and 3) ashes have low solubility and, thus, are incorporated to the cellulose stream. The previous formulas used to calculate hydrogen contents and higher heating values are accordingly adapted as follows:

$$H_{NFF} = \frac{f}{\sum c_k} . (c_2 . H_2 + c_3 . H_3) + s . H_{sucrose} \tag{15}$$

$$HHV_{NFF} = \frac{f}{\sum c_k} . (c_2 . HHV_2 + c_3 . HHV_3) + s . HHV_{sucrose} \tag{16}$$

Heat generated from bagasse combustion is converted into electricity through a thermodynamic power cycle, which allows sugarcane processing plants to be energetically self-sufficient and to sell surplus electricity to the grid. The efficiency of this conversion operation is commonly defined as a percentage of the lower heating value of the fuel consumed, typically about 33% to 48%. This efficiency is limited by the 2nd law of thermodynamics which states that "…no process is possible in which the sole result is the absorption of heat from a reservoir and its complete conversion into work…" (Kelvin's statement). Therefore, some amount of heat must be rejected so that the cycle is physically possible. Because in the process there are several applications that require heat (distillation, juice reduction, etc.), the cycle's waste heat can be captured and distributed locally to achieve higher overall energy efficiencies. This is known as combined heat and power generation, or simply cogeneration.

3. NUMERICAL SIMULATIONS AND RESULTS

The industrial conversion of biomass is influenced by two types of variables. Control variables, such as boiler pressure or distillation temperature, are the ones that can be set by the operator. Other intervening variables are stochastic in nature and cannot be controlled by the operator. For simplicity, some variables will be considered deterministic in nature and will be set as parameters of the conversion model. All variables and parameters of the simulations performed in this work are defined in Tab. 4, together with their corresponding types and random limits.

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Table 4. Simulation variables and ranges used in simulations

variable	**symbol**	**lower limit**	**upper limit**	**unit**	**type**
1G ethanol	$\dot{m}_{1G}$	53.75	53.75	m^3/h	deterministic
electricity from straw	W_{str}	7.53	7.53	MW	deterministic
rate of burning bagasse	$\dot{m}_{bg}$	0	150	t/h	uniform random
fiber content	f	35	40	%	uniform random
water content	w	45	60	%	uniform random
sucrose content	s	0	1	%	uniform random
ash content	a	0	20	%	dependent random
cellulose content	c_1	3	4	parts	uniform random
hemicelluloses content	c_2	2	3	parts	uniform random
lignin content	c_3	1	2	parts	uniform random
cellulose yield	η_{cell}	0.88	0.92	kg/kg	uniform random
hemicelluloses yield	η_{hcell}	0.80	0.90	kg/kg	uniform random
lignin yield	η_{lign}	0.90	0.95	kg/kg	uniform random
cellulose to glucose eff.	η_{gluc}	0.75	0.95	kg/kg	uniform random
glucose to ethanol eff.	η_{geth}	0.90	0.95	kg/kg	uniform random
hemicellulose to xylose eff.	η_{xylo}	0.60	0.90	kg/kg	uniform random
xylose to ethanol eff.	η_{xeth}	0.65	0.90	kg/kg	uniform random

A particular set of values assigned to these variables results in specific values of the output energy vectors and is represented as a unique operating state in the ethanol-electricity graph, also called state diagram (Fig. 4). The ensemble of all possible states defines the so-called process operating envelope which is delimited by three curves: 1) first generation ethanol production from juice, 2) electricity production from straw and 3) energy limit imposed by the energy conservation principle (Pareto frontier). From a conversion efficiency perspective, the operator's main concern is to set the control variables so that the process state is always near the Pareto frontier, i.e. within the target operating region, no matter the stochastic variations of fiber content, bagasse humidity, residual sucrose, cellulose content, etc. The point is to set the control variables to obtain increased probabilities of getting operating states in the target operating region.

This can be done by comparing the process variables' probability density functions (pdfs) corresponding to operating states lying in the operating target region, near the energy limit, and all other states in the operating envelope. These pdfs contain extremely rich and useful information, not only to the more immediate decisions regarding the industrial conversion process, but also to mid and long term planning related to agricultural production and feedstock logistics. For instance, it can be speculated that less lignin is better because its fermentation is still not feasible at scale. But on the other hand, its energy content is more than twice the energy contents of cellulose and hemicelluloses and, consequently, as far as electricity production is the main concern, it is more advantageous to cultivate sugarcane varieties with higher lignin contents.

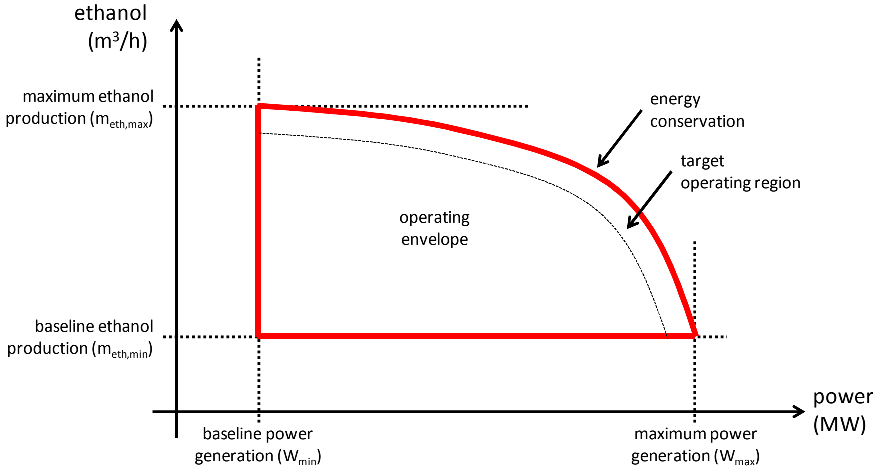

Figure 4. Ethanol-electricity graph (state diagram) and process operating envelope

Considering the scope of this work, we will neglect the stochastic variability imposed by variables related to the existing process, which will for now on be considered as fixed parameters. As already mentioned, these deterministic parameters constitute the ethanol and electricity generation baselines of the operating envelope in Fig. 4, respectively 53.75 m^3/h and 7.53 MW. The upper limit or the Pareto frontier of the operating envelope is determined by the energy conservation principle: the energy content of the produced energy vectors is limited by the energy content of the feedstock, all conversion efficiencies considered. In our simulations these limits were not imposed a priori, but extracted from the states in the ethanol-electricity plot. This was accomplished by identifying the convex hull encompassing all state points. Specifically, we applied the "gift wrapping" algorithm described by Borgwardt (1997). The target operating region's lower limit (dotted line in Fig. 4) was defined by fitting a polynomial curve to a shrinked version of the Pareto frontier. That is, if $(W_{tb}, \dot{m}_{eth})$ are points of the Pareto frontier, we fitted a fourth order polynomial to the points $(x \cdot W_{tb},\ x \cdot \dot{m}_{eth})$, where the scale factor x was set at 98.5%.

Since our problem has several coupled degrees of freedom, which makes any deterministic algorithm impractical, we performed Monte Carlo experiments by feeding pseudo-random values to the conversion model and deterministically calculating the output energy vectors from the equations described previously. The state diagrams for two distinct conversion routes in which hemicelluloses are exclusively burned or fermented are shown in Fig. 5. As dictated by the energy conservation principle, electricity generation is directly proportional to the rate of burning bagasse while ethanol production is inversely proportional to it. Linear regression formulas for both hemicelluloses' pathways are:

$$W_{tb} = 14.02 + 0.17 \cdot \dot{m}_{bg} \tag{17}$$

$$\dot{m}_{eth} = 76.04 - 0.14 \cdot \dot{m}_{bg} \tag{18}$$

where m_{in} is in [t/h] and W_{tb} in [MW]. An important information that can inferred from these equations is related to the average conversion maxima/minima of electricity generation and ethanol production. These values are 40 MW @ m_{bg} = 150 t/h and 76.04 MW @ m_{bg} = 0, respectively. Comparing these values with those of a typical 1G sugarcane processing plant which is capable of converting 500 tsc/h into 43 m^3/h of ethanol and 50 MW of electricity (2.2 MPa, 100kWh/tsc), it is possible to note that the overall conversion efficiency is greatly improved due to the 2G conversion pathway, all stochastic variations considered.

The graphs in Fig. 5 show that fermenting hemicelluloses increases ethanol production while electricity generation is practically unchanged. This is so because of two important effects caused by the introduction of the 2G ethanol production process: 1) energy consumption in dewatering biomass fuel previously to burning is reduced and 2) heating value of biomass fuel is increased due to higher contents of lignin.

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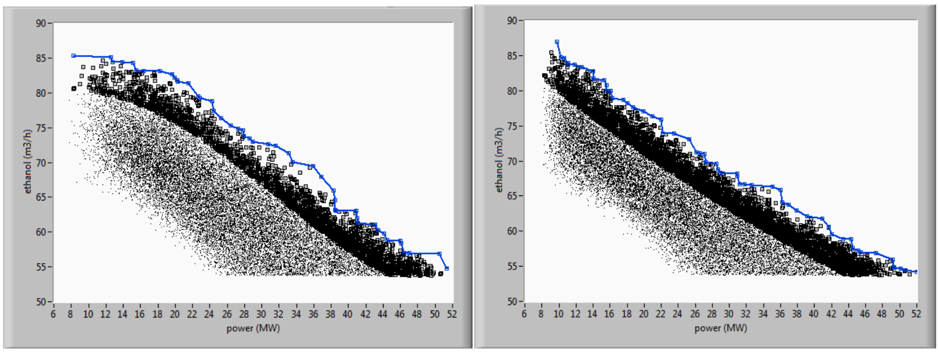

Figure 5. Operating state diagrams for two hemicelluloses conversion pathway: (a) hemicelluloses are burned, (b) hemicelluloses are fermented. Legend: □ = Pareto frontier, ⊡ = target operating region and (·) = general operating states

Optimum conversion efficiencies are achieved when the states of the process lay within the target operating region as shown in Fig. 5. The specific characteristics of the stochastic variables that result in optimality can be inferred from the corresponding pdfs shown in Figs. 5 to 10. To begin with, optimum operation is greatly affected if hemicelluloses are burned or fermented. In the first case, the difference between the envelope and the target states pdfs (Fig. 5 – left) indicates that optimality is strongly related to the rate of burning bagasse. Most likely optimal operation occurs around 20MW and 43MW which corresponds rates of burning bagasse of approximately 35.1 t/h and 170.5 t/h respectively. These two peaks are consistent with ethanol production (Fig. 5 – right) in the sense that they correspond to the same rates of burning bagasse for which ethanol production is optimal. However, optimal operation at 35.1 t/h is achievable, although less likely, for all possible values of the stochastic variables, while the second one is occurs only for a small subset of them. In other words, 43 MW occurs only for special values of bagasse composition, humidity, cellulose content, etc., that compensate the fact that the maximum amount of burning bagasse is 150 t/h.

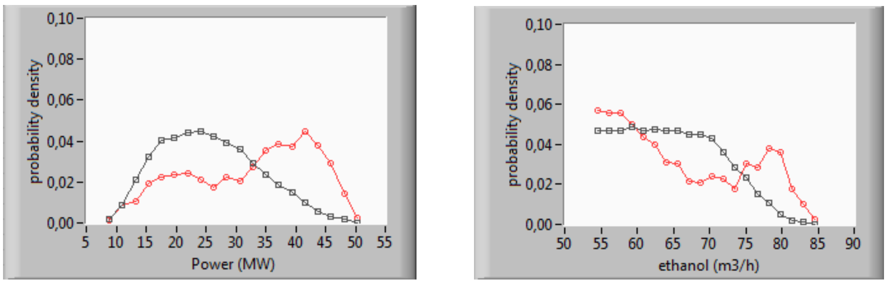

Figure 5. Power and ethanol probability density functions within the operating envelope (□) and in the optimum target region (○) – hemicelluloses are burned

In contrast with that, when hemicelluloses are fermented (Fig. 6) the differences between these pdfs are less pronounced. In fact, both optimal electricity and ethanol pdfs in Fig. 6 resemble more closely a uniform distribution what means that optimal operation is less sensitive to variations of the uncontrolled variables and, consequently, the process is much more robust. The explanation for this is related to the intrinsic characteristics of hemicelluloses in terms of its conversion into an energy vector: a relatively low heating value (compared with lignin) and good yield and fermentation efficiencies.

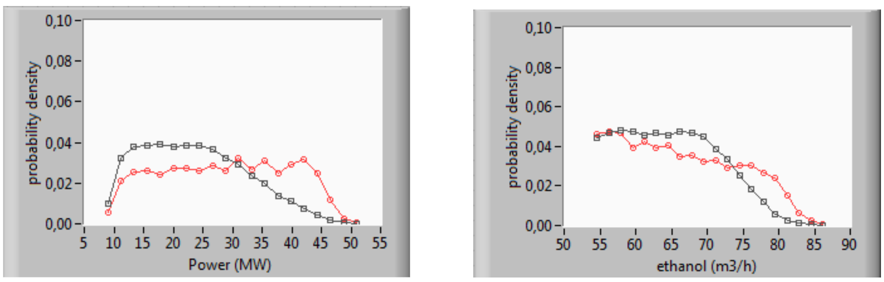

Figure 6. Power and ethanol probability density functions within the operating envelope (□) and in the optimum target region (○) – hemicelluloses are fermented.

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The biomass constitution variables are bagasse fiber and water contents and, in addition, fiber constitution in terms of cellulose, hemicelluloses and lignin. The pdfs of the first two ones are shown in Figs. 7 and 8, both for burning and fermenting hemicelluloses. The results are as expected: optimal operation is more likely to be achieved if bagasse has higher fiber contents and lower humidities. This is so because fiber is rich in energy, which can be converted into electricity or ethanol, and because water demands energy to be dewatered, in addition to lowering biomass fuel's heating value. However, water content pdfs also imply that fermenting hemicelluloses is a much more robust conversion process in terms of admitting higher humidities at the target operating region. This is explained by the fact that smaller amounts of biomass fuel have to be dewatered previously to burning, even though they are richer in energy because of its higher lignin content. Additionally, optimal operation is very unlikely for both conversion routes at humidities above 53% within the operating conditions previously set.

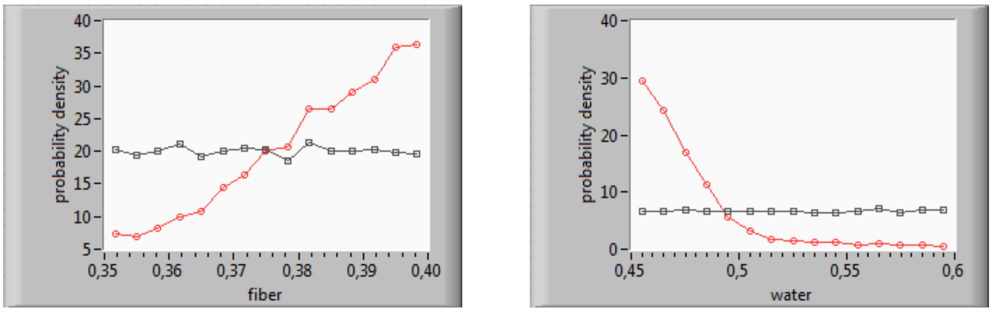

Figure 7. Fiber and water contents probability density functions within the operating envelope (☐) and in the optimum target region (○) – hemicelluloses are burned.

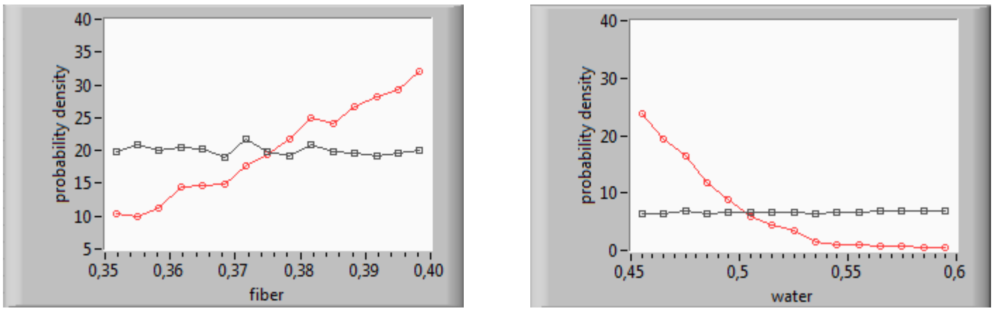

Figure 8. Fiber and water contents probability density functions within the operating envelope (☐) and in the optimum target region (○) – hemicelluloses are fermented.

Fiber constitution also has significant effects on optimality and robustness of the industrial conversion process. It can be inferred from the corresponding pdfs that, if hemicelluloses are burned to generate power, maximum probabilities of achieving the target operating region result from a 3:3:2 composition in terms of cellulose, hemicelluloses and lignin respectively (Fig. 9). This is again a consequence of the fact that lignin has a higher heating value compared with the heating values of cellulose and hemicelluloses. Consequently, biomass fuels richer in lignin are more likely to result in states within the target operating region. Conversely, if hemicelluloses are fermented to produce ethanol, the effect of biomass composition has a smaller effect on optimality of the conversion process, as it can be inferred from the pdfs shown in Fig. 10. Since biomass composition varies stochastically due to soil composition, climate conditions, etc., fermenting hemicelluloses constitutes a much more robust conversion route, what corroborates the importance of developing efficient methods for fermenting C5 sugars.

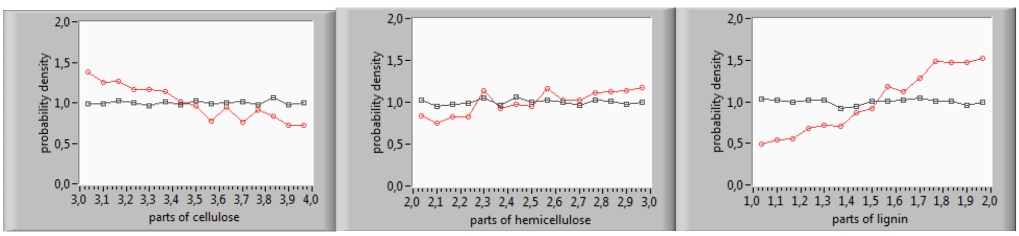

Figure 9. Fiber components probability density functions within the operating envelope (☐) and in the optimum target region (○) – hemicelluloses are burned.

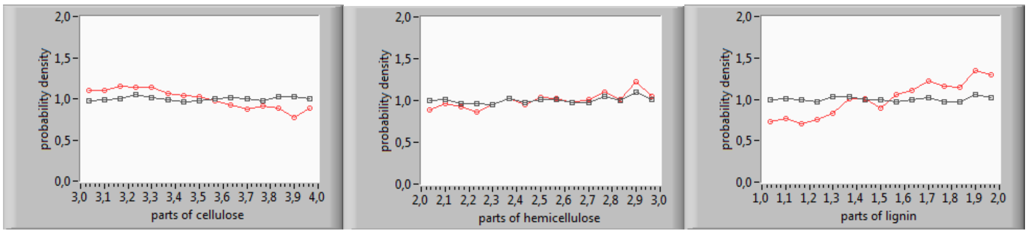

Figure 10. Fiber components probability density functions within the operating envelope (□) and in the optimum target region (○) – hemicelluloses are fermented.

4. CONCLUSIONS

This work presented a multi-objective optimization study of the industrial conversion of sugarcane into energy vectors, considering the integration of a 2nd generation ethanol production pathway. The main objective was determine new optimized operating conditions and to statistically characterize its corresponding operating variables. A reference sugarcane industrial processing plant was set and a comprehensive model describing all its unit operations and chemical reactions was simulated by the Monte Carlo method. A total number of 20,000 experiments were simulated by assigning uniform random values to 15 variables of the conversion model to determine the resulting electricity generation and ethanol production. Specific values of the output energy vectors define the operating state of the process and the ensemble of all possible states defines the so-called process operating envelope in the ethanol-electricity graph (state diagram). The operating envelope is upper bounded by the principle of energy conservation which is materialized by the conversion energy limit or Pareto frontier. From a conversion efficiency perspective, the operator's main concern is to set the control variable (rate of burning bagasse) in order to operate near the Pareto frontier independently of stochastic variations on fiber content, bagasse humidity, residual sucrose, cellulose content, etc., as shown in Fig. 5.

Results show that input variables have specific characteristics when their operating states lye near the energy limit. By analyzing their probability density functions (pdfs) it is possible to conclude that simultaneously optimal ethanol production and electricity generation occur at low burning bagasse rates (Figs. 5 and 6), basically due to relatively high energy demands of the dewatering operation compared with the 2nd generation ethanol pathway for which it is not necessary to dewater the fermentable biomass fractions. Hemicelluloses' pdfs in Figs. 9 and 10 also reveal important information about its conversion pathway, i.e. through fermentation or combustion. Because of its relatively low heating value (compared with lignin) and good yield/fermentation characteristics, fermenting hemicelluloses, instead of burning it, increases the probability of optimal operation near the maximum energy conversion limit. Additionally, this alternative results in a more robust process in the sense that optimality is less sensitive to fiber composition and water content (Fig. 8). Finally, if hemicelluloses should be burned, it is better to have feedstocks richer in lignin because of its higher energy content as it can be inferred from lignin's pdfs in Figs. 9 and 10. Furthermore, it is plausible to suppose that higher lignin contents results in more regular sugarcane stalks which are likely to be harvested more efficiently.

These are extremely rich and useful information, not only to the more immediate decisions regarding the industrial conversion process, but also to mid and long term planning related to agricultural production issues as well as equipment development and feedstock logistics. To conclude, although the analysis was based on the sugarcane processing industry in Brazil, the same approach is applicable to other agricultural crops in other countries.

5. ACKNOWLEDGEMENTS

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