



Acetone, Butanol, Ethanol and, Xylitol Production Through a Biorefinery Platform: An Experimental & Simulation Approach

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Abstract

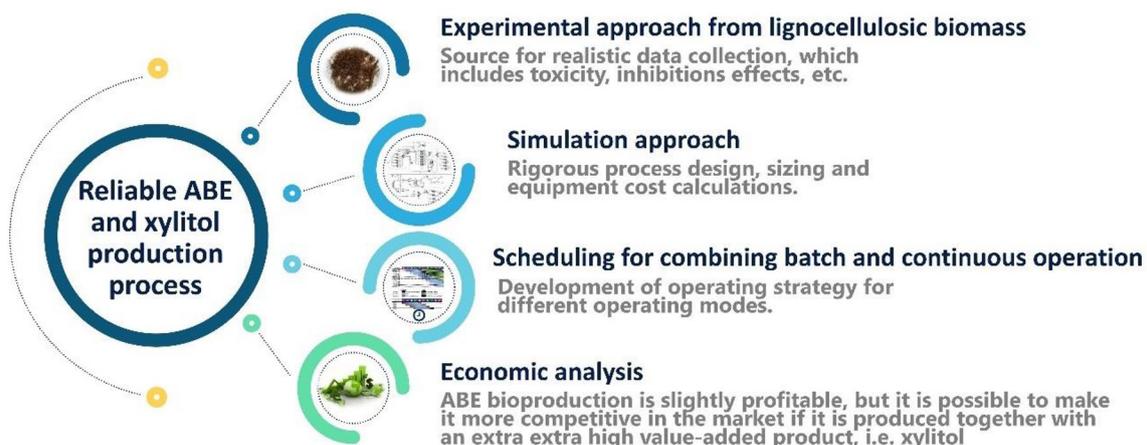
Purpose Butanol is an interesting biofuel and a product precursor, that could be obtained with acetone and ethanol via fermentation. The biofuels production has been identified as not economically competitive, thus, the parallel production of high value-added products, such as xylitol, could be an alternative to improve the profit. Xylitol can be produced from xylose, which might be considered as a coproduct in a second generation biorefinery.

Methods This study presents a systematic biorefinery process design for the simultaneous acetone, butanol, ethanol (ABE) and xylitol production, based on experimental and simulation approaches. Experiments were performed for the pretreatment of sugarcane bagasse and ABE fermentation. The simulation part used the experimental results and experimental data from literature, to perform rigorous calculations of the ABE and xylitol production process. The economic analysis (EA) was performed relying on some indicators such as, the net present value (NPV) and payback period (PBP); EA includes several scenarios for producing only ABE and some scenarios for simultaneous ABE and xylitol production.

Results The results showed that the combined butanol and xylitol production could reduce by 17% the selling price of butanol, compared with only producing butanol. The study also included the combustion of residual solids and carbon dioxide depletion analyses.

Conclusion This approach illustrates the opportunity to perform a rigorous techno-economic analysis, to identify the feasibility of the process at industrial scale, based on realistic data. This approach was implemented for ABE and xylitol production, but it can be used to any other bioproduct.

Graphic Abstract



Keywords ABE · Xylitol · Energy transfer · Value-added products · Profit · Net present value

Extended author information available on the last page of the article

Abbreviations

ABE	Acetone, butanol and ethanol
BO	Batch operation
BT	Bottom temperature
CC	Cellulose conversion
CO	Continuous operation
DB	Dry bagasse
EH	Enzymatic hydrolysis
FLP	First liquid phase
FS	Feed stage location
G	Glucose
GC	Glucose conversion
HB	Humid bagasse
HC	Hemicellulose conversion
IRR	Internal rate of return
KC	Key compound
NPV	Net present value
NS	Number of stages
P	Pressure
PBP	Payback period
PC	Partial condenser
PI	Pressure increase
PT	Pretreatment
ROI	Return of investment
RR	Reflux ratio
RT	Reacting time
SAC	Sulfuric acid conversion
SLP	Second liquid phase
T	Temperature
TT	Top temperature
VS	Vessel size
VN	Vessels number
XC	Xylose conversion

Statement of Novelty

The work presents a systematic process design for acetone, butanol, ethanol (ABE) and, xylitol production in a biorefinery platform. The design includes some experiments, which were useful to guide and obtain realistic process conditions to subsequently carry out the rigorous simulation of the process. The study performs a techno-economic analysis, to verify the positive impact of producing xylitol together with ABE. The results illustrate a significant reduction in the butanol selling price, making it more competitive against the butanol produced from crude oil. The study also includes the analysis of combusting the residual solids at the biorefinery and the impact from the economic and environmental point of view. To the best of our knowledge, it has not been published a similar work in the existing journals. Thus, we consider this manuscript will highly contribute to the state of art related with biofuels production, especially, for the

butanol production. The reader will finally verify with the performed analysis, that biofuels production cost could be decreased when it is produced simultaneously with a high value-added product.

Introduction

The production of biofuels and high value-added products from lignocellulosic biomass has gained special interest, due to the possible reduction of crude oil production and the greenhouse effects in the environment. Besides, biofuels have also been identified as an important part of the future energy supply, mainly for the transportation sector [1]. There are several biomass-based biofuels such as, bioethanol, biomethanol, biosyngas, biobutanol, etc. Among the different products from lignocellulosic material, butanol has shown to be advantageous as a potential biofuel, for example, compared with ethanol, the energy content of butanol is higher and the vapor pressure is lower for butanol; both properties facilitate its use in existing gasoline supply and distribution channels; moreover, butanol can be blended easily with gasoline, and it is less hydrophilic compared to bioethanol [2]. Butanol has also been investigated as a precursor in the fuel sector to produce biogasoline, jet fuel and biodiesel [3], additives for biodiesel, and hydrogen by reforming butanol [4].

The acetone, butanol and ethanol (ABE) production process employing lignocellulosic biomass includes four main sections. 1) pretreatment (PT): the main objective is breaking down the lignocellulosic matrix, to make the cellulose available for the hydrolysis step; 2) enzymatic hydrolysis (EH): this section employs enzyme cocktails including some cellulases, which liberate the remaining glucose from the polysaccharide chain of the pretreated biomass; 3) ABE fermentation: the glucose is metabolized by the microorganisms to produce acetone, butanol and ethanol; 4) downstream process: the main purpose of this section is the purification of butanol and high valued-added products, as well as the recovery of some reactants.

The first and second sections of the process are similar to the lignocellulosic ethanol production process [5–7]. Butanol production by a biotechnological pathway has been performed employing bacteria from the genus *Clostridium*, such as *Clostridium acetobutylicum* and *Clostridium beijerinckii*, among others [8–10]. The simultaneous ABE production could be an advantage, due to the diverse products from the fermentation. However, it could also be a disadvantage, because that would increase the complexity in the separation and purification process. Besides, the low concentrations of ABE in the fermentation broth, has been identified as one of the main drawbacks of this process, because that could affect its profitability.

Regarding to the purification and separation processes for ABE, several studies have tried to employ and combine diverse separation technologies to overcome those issues: Heitmann et al. [11] performed a simulation to compare three separation process configurations for a hypothetical binary water-butanol mixture, where the authors proposed the use of heteroazeotropic distillation, integrated extraction-distillation using an ionic liquid, and an integrated pervaporation-distillation process. On the other hand, using a similar representative mixture, Luyben [12] also proposed and simulated a heteroazeotropic distillation process, but at vacuum conditions for one of the distillations columns. Kraemer et al. [13] simulated the separation of acetone, butanol, ethanol and water leaving the fermenter, using a hybrid extraction-distillation that consisted of an extraction process using an organic solvent (1,3,5-trimethylbenzene) for ABE, and a train of three distillation columns. Besides, Errico et al. [14] proposed new hybrid process configurations, which showed a variety of options to this end. Anbarasan et al. [3] relying on an experimental approach, proposed the removal of ABE with liquid–liquid extraction using glyceryl tributyrate as an extractant, followed by a hypothetical distillation process. On the other hand, Qureshi et al. [15] presented a collection of experimental studies for butanol recovery mostly from a water-butanol mixture, employing adsorption to separate butanol. Other studies have proposed the use of gas stripping for in situ removal of ABE from the fermentation broth, for instance, employing nitrogen [16]. There are several technology options for the purification and separation of the products of the ABE process, but most of the previous works have considered a hypothetical mixture using the main compounds of the fermentation broth, such as, a butanol-water binary mixture or a blend containing acetone, butanol, ethanol and water, which could be a close approximation to the real mixture, but the presence of other compounds leaving from the fermentor (e.g. not converted sugars, carbon dioxide and hydrogen) can really introduce a difference in the thermodynamic behavior of the downstream processes.

Moreover, it has been shown that a single product process is not completely worthwhile, thus, it has been proposed the supplementary production of electricity and high value-added products such as lactic acid, succinic acid, mannitol, xylitol, etc. in order to make a cost-effective process [17–19].

The industrial production of xylitol is carried out reducing pure xylose, in the presence of a metallic catalyst at elevated temperatures (373–418 K) and pressures (up to 5,060 kPa) [20, 21]. On the other hand, recent research has focused on the biotechnological production through fermentation process by yeast, including genera *Saccharomyces*, *Candida*, *Meyerozyma* and *Pichia*. Xylitol production has the advantage that could be produced from the diaxix

conversion of xylose and glucose, which are residues from lignocellulosic biomass-based bioprocesses [22, 23].

Santibañez-Aguilar et al. designed biorefinery supply chains under uncertainties for the Mexican scenario, showing that the simultaneous butanol, ethanol and xylitol production were feasible to be produced in a distributed biorefinery system [24]. Besides, the high production of lignocellulosic residues in Mexico, illustrates the potential production of biofuels and high value-added products. For example, the sugarcane bagasse is one of the residues from sugar production, that could be efficiently used for bioproducts production, especially in the State of Veracruz where the sugar industry is mainly located.

In the past years, the research activities regarding to ABE and xylitol production processes, have been mostly performed studying the different sections of the process separately, which can provide relevant information; but the successive and integral analysis for these processes must be performed.

Thus, the objective of this work is to present a process design and operation strategy for the simultaneous acetone, butanol, ethanol and, xylitol production in a biorefinery platform, including some tasks from the experimental, simulation and model-based approaches.

Materials and Methods

The development of this study relied on two principal parts: the collection of experimental data [25] and the simulation activities. The first part consisted on the biomass selection and characterization, selection of the concentration and type of acid employed in the pretreatment, determination of the degree of conversion in the fermentation process and, the selection of the proper operating conditions for the pretreatment and fermentation unit. The process structure of the simulation in the ABE production was mainly based on previous works [5–7, 10].

Experimental Approach

The experimental activities were performed in a lab scale.

Lignocellulosic Raw Material Characterization

The sugarcane production company “Central Motzorongo” located in Veracruz state provided the raw material employed in this work. The study included two types of bagasse: the bagasse obtained after the sugar extraction (dry bagasse, DB) and the dry bagasse mixed with urea that is usually destined for animal feed (humid bagasse, HB). The content of cellulose, lignin and hemicellulose were determined using the method reported by Abdullah et al. [26].

Pretreatment Section

Both types of sugarcane bagasse were dried during 24 h at 68 °C, afterwards, the solids were grinded until getting an average particle size of 0.64 mm. The pretreatment of the sugarcane bagasse was performed at different temperatures (100, 110 and 120 °C) and sulfuric acid concentrations (0, 2, 4, 6, 8, 10% wt/wt). The pretreatment was carried out in an autoclave. Similarly, to some previous works [27, 28], for the reaction time, 5 min were counted once the desired temperature was reached in the autoclave, followed by an immediate decompression and the cooling of the sample in an ice bath. The liquid and solid phases were separated using filtration with filter paper and neutralized with sodium hydroxide. The liquid phase was used to measure the reducing sugars concentration [29] and, perform the toxicity analysis to verify whether the medium could inhibit the microorganism growth.

For the toxicity analysis, *Clostridium acetobutylicum* CDBB 797 was used, which was obtained from the national collection of microbial strains and cell cultures in Mexico [30]. *C. acetobutylicum* CDBB 797 was inoculated at 10% and grown in a medium containing (g L⁻¹): casein peptone, 10; yeast extract, 3; and carbon source, 10. Treatment media containing pretreated liquid phase and glucose were compared to control medium, which only contained glucose. The growth of the microorganism was analyzed by spectrophotometry. More details about the experimental steps could be found in the literature [25, 31].

ABE Fermentation

Clostridium acetobutylicum CDBB 797 was inoculated with 10% v/v active proliferating bacteria (24 h grown) from pre-inoculum medium. The cultivation was done using 50 g L⁻¹ of glucose. The medium was sterilized in the autoclave, and then biotin and p-aminobenzoic acid (1 mg L⁻¹) were added to the medium by filtration using 0.1 µm pore membrane. The fermentation was carried out during 233 h at 37 °C, with initial pH of 5. The anaerobic conditions were set by injecting nitrogen. A sampling schedule was used to determine the glucose and products concentration. More details about the experimental steps have been published previously [25].

Analytical Methods

Reducing Sugar Concentration The concentration of reducing sugars from the pretreatment and the substrate consumption during fermentation, were determined using the method proposed by Miller [29]. The ELx808™ Absorbance Microplate Reader at 540 nm was used for the measurements. A standard curve with glucose standard solutions was employed for the quantification [32].

Cell Growth Analysis in Toxicity Test The toxicity analysis was done comparing the estimated cell growth of *C. acetobutylicum* in the control (glucose) and pretreatment liquid phase (treatment) media by measuring the optical density at 560 nm, with a spectrophotometer UV–VIS Genesys 10 S (Thermo Scientific, USA).

Acetone, Butanol and Ethanol Quantification The acetone, butanol and ethanol concentration were determined with a chromatograph (Agilent model 7820), equipped with a flame ionization detector (FID) and an Innowax column (Agilent). According to Tashiro et al. [33], the oven temperature was programmed to increase from 50 °C to 170 °C, at the rate of 10 °C min⁻¹. The injector and detector temperatures were set at 250 °C. Helium was the carrier gas and a flow rate of 3.7 mL min⁻¹ was used during the detections. Commercial acetone, butanol and ethanol standard solutions, were employed to identify the retention time and to set the calibration curve.

Statistical Analysis Data were statistically analyzed by analysis of variance (ANOVA) using the software SPSS 13 for windows, (IBM, NY, USA, 2004). Significance was $p < 0.05$ and least significant value by Tukey test was used to identify groups.

Computational Section

The methodology followed in this study (see Fig. 1) consists of three main stages: data collection, simulation, data analysis and the evaluation of the process configuration.

Data Collection

This stage started with the collection of the necessary information such as, the composition of the raw material, the possible compound that could be produced in a chemical or biochemical reaction, as well as the potential technologies and operating conditions from literature or lab results. The next step was to determine the appropriate thermodynamic models, to be employed in each unit operation of the process.

Simulation and Data Analysis

The second stage consisted on the evaluation of process configurations relying on previous studies aiming to be improved, or propose new process configurations including the design of a conventional unit operation, intensified units, or the use of hybrid processes. The design of the unit operations starts employing shortcut methods,



Fig. 1 Methodology for the simulation approach

followed by rigorous simulation. Here, previous literature results or those obtained at lab scale, were employed as process conditions. Aspen plus v 8.8 was used to perform the simulations.

Economic Analysis of Process Configuration

The last stage is to compare the process configurations to select the most promising of them, in terms of the established benchmarking criteria. The benchmarking criteria were based on some economic indicators: net present value (NPV), internal rate of return (IRR) and the payback period (PBP). The selected criteria allowed analyzing the profitability of the process configuration evaluating the selling cost of the products. The economic analysis was performed employing the Aspen Economic Analyzer v 8.8. The cost of the equipment and utilities correspond to February 2020.

Results and Discussion

Experimental Approach

Pretreatment

The pretreatment experiments allowed the selection of process conditions to be evaluated in the simulation steps. The results of the pretreatment are illustrated in Fig. 2a. The highest yield for sugars obtained from the dry bagasse (0.2 ± 0.01 g reducing sugars g^{-1} of bagasse), was found

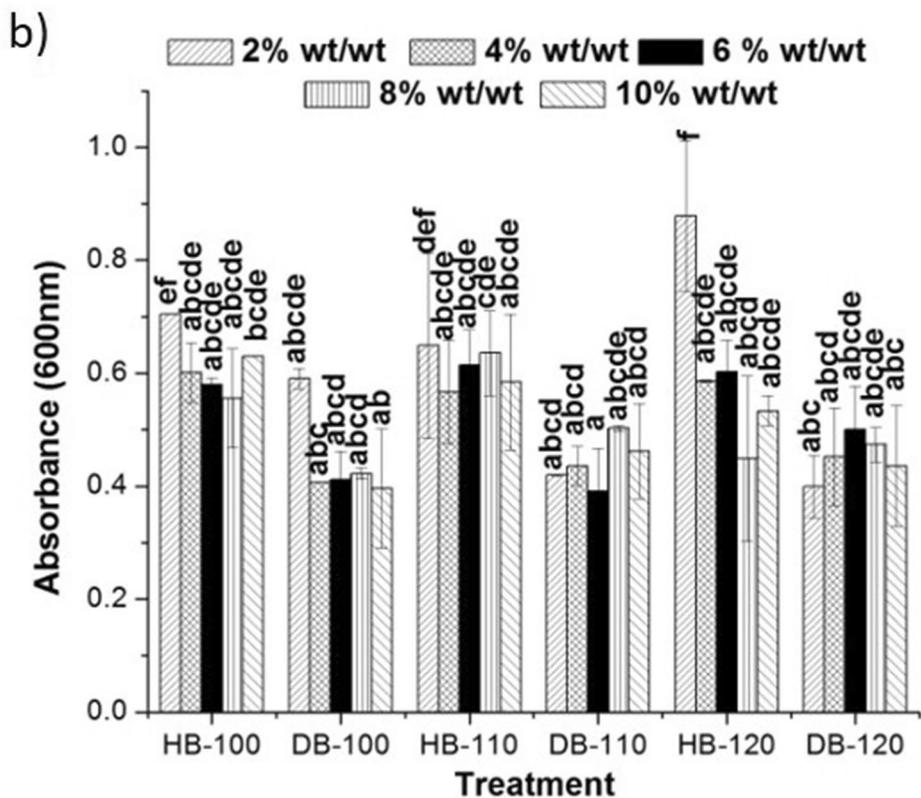
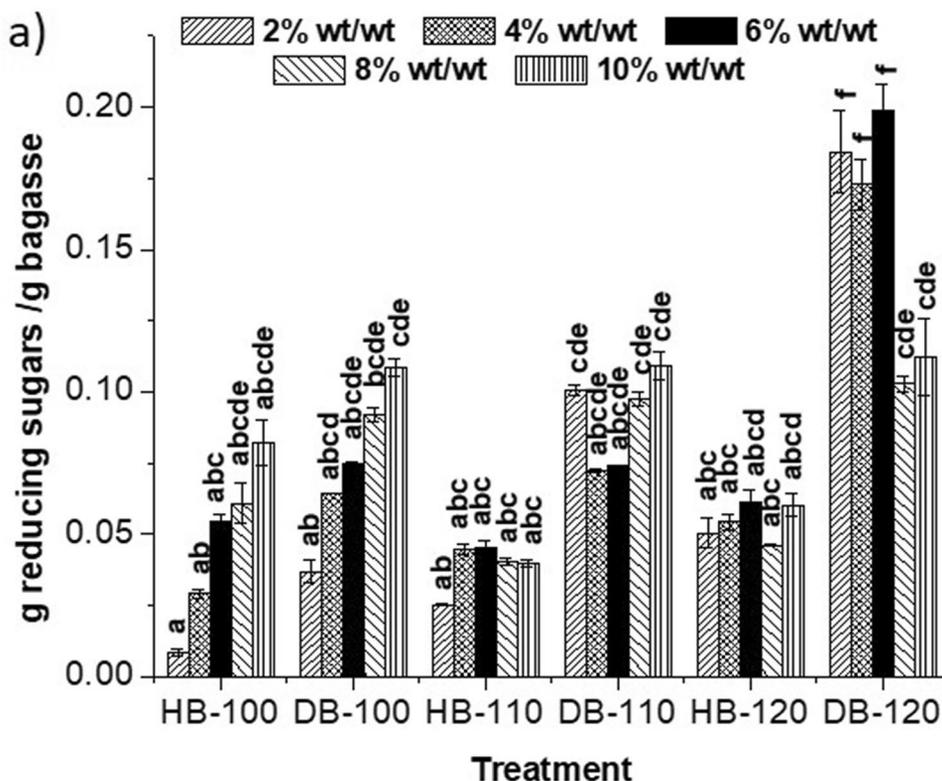
at the temperature of 120 °C and acid concentration of 6% wt/wt. Regarding to humid bagasse, the best results (0.08 ± 0.01 g reducing sugars g^{-1} of bagasse) was found at the temperature of 100 °C and 10% wt/wt of acid concentration. When comparing humid and dry bagasse, the highest reducing sugars release was always observed in the liquid fraction of pretreated dry bagasse, except at 100 °C that no significant differences were observed. Thus, the liquid phase product of the pretreatment at 120 °C and acid concentration of 6% wt/wt, was selected to be used in subsequent experiments and, the process conditions in the simulation part. The conversion from cellulose to glucose at the selected conditions was 27.65%, which is also used in the simulation part. It was assumed that the main reducing sugar was glucose.

The toxicity analysis showed that there was not growth inhibition of *C. acetobutylicum*, owing to the released compounds from the pretreatment section. Figure 2.b shows that the absorbances in all tested media were equal or higher than the obtained in the control medium ($A=0.3$). There was not significant difference in the absorbance measurements among all media (0.3–0.7), except for medium supplemented with pretreated liquid from humid bagasse at 120 °C ($A=0.9$).

Fermentation

Fermentation of *C. acetobutylicum* was performed using glucose as substrate, since the toxicity analysis did not show growth inhibition related to the presence of toxic compounds in the pretreated liquid phase. The final concentrations of the

Fig. 2 a Reducing sugars released from sugarcane bagasse pretreatment at different temperatures and acid concentration. **b** Absorbance of *Clostridium acetobutylicum* grown on liquid fraction of pretreated sugarcane bagasse obtained at different temperatures and acid concentrations. Humid bagasse (HB) and dry bagasse (DB) at 100, 110 and 120 °C, 2 to 10% sulfuric acid solution. Different superscript letters are statistically different ($p < 0.05$, Tukey’s test)



acetone, butanol, ethanol, and biomass were 3.4, 7.65, 1.33 and 1.88 g L⁻¹, respectively; and the corresponding substrate consumption was 89.7%, which was determined using the DNS method [29].

Simulation Approach

Data Collection

ABE Production The first step is the collection of data that was mostly obtained from experimental approach, such as, temperatures and pressure conditions in the unit operation, percentage conversion of reactants, compositions entering and leaving the operation unit, among others; in addition, with some data from the literature.

The process conditions extracted from experiments for the pretreatment were the conversion of cellulose to glucose (27.65%), operating temperature (120 °C) and sulfuric acid concentration (6% wt/wt). The operating conditions for the enzymatic hydrolysis were obtained from a previous publication [34]. The temperature proposed in the publication was 50 °C, pressure of 1 atm with a cellulose to glucose conversion of 66%. The collected information from the fermentation was the operating temperature (37 °C), fermenter pressure (1 atm) and the glucose conversion into ABE products (89.7%). Regarding to xylose conversion to ABE, some studies [35, 36] have shown that xylose consumption is not significant in the presence of glucose, thereby, due to glucose was not totally consumed during the fermentation, it has been assumed that xylose was not consumed in the ABE fermentation.

Regarding to separation and purification processes of ABE, Errico et al. [14] truly gives an extensive number of alternatives, where the liquid–liquid separation followed by three distillation columns was selected for the downstream processes.

Xylitol Production In a previous work for bioethanol production [5], the waste stream of the bioethanol production process consisting of the residual xylose was employed to produce xylitol. Thereby, a similar analysis was performed in this study. The process conditions for the xylitol production reactions were 303.15 K for the operating temperature and 1 atm of pressure, in aerobic conditions employing the yeast *Candida mogii* ATCC 18364 [23]. The glucose consumption and the conversion of xylose to xylitol in the fermentor were determined using the model proposed by Tochampa et al. [23], which considers xylose and glucose as carbon sources in the fermentation. The values for the initial xylose and glucose concentrations to perform the calculations in batch mode, were obtained from the stream of the process containing the residual sugars. The initial glucose and xylose concentrations were 8.92 g L⁻¹ and 2.38 g

L⁻¹, respectively; and the initial microorganism concentration was 3 g L⁻¹. The calculated conversion for glucose was 100% and 79% for xylose. The modelling also allowed determining the time of the maximum conversion to estimate the size of the fermenters. The modelling task was done using Matlab® v. 7.9.

Thermodynamic Model Selection The phase equilibria and thermodynamic properties were calculated using the NRTL model [37] and the Hayden-O'Connell equation of state [38]. The parameters of the NRTL model to simulate the pretreatment, enzymatic hydrolysis and fermentation sections were taken from previous studies [7, 39]. Regarding to the separation and purification process, the parameters employed in the NRTL model were also collected from previous works [14, 40].

Treated Mass and Chemical Composition of Raw Material In order to carry out a realistic simulation, the capacity of the plant was calculated considering a certain demand of biobutanol in Mexico, to blend with gasoline and cover part of the daily consumed fuel [41]. The biobutanol demand calculated was 103,876.00 kg d⁻¹. Thus, knowing the amount of required biobutanol and using the data collected from the experiments, it was possible to calculate the required amount of sugarcane bagasse to be processed to produce the biofuel demand. The amount of sugarcane bagasse to be treated was 693,278.00 kg d⁻¹.

The sugarcane bagasse dry compositions for cellulose, hemicellulose, lignin and ash were 72.33%, 2.75%, 15.75% and 9.17%, respectively. The composition was calculated as proposed by Abdullah et al. [26].

Simulation and Data Analysis

The simulations and calculations of the process were performed in Aspen Plus v. 8.8, employing the collected data and some information from previous studies [6, 7, 34]. The Fig. 3 illustrates the process configuration proposed for the ABE and xylitol production in a biorefinery platform. The flowsheet includes 7 sections: 1) pretreatment, 2) neutralization and nutrient production (nitrogen source), 3) enzymatic hydrolysis, 4) seed culture, 5) ABE fermentation section, 6) downstream process for acetone, butanol and ethanol, and 7) xylitol production and purification.

The design details of the unit operations are illustrated in Table 1. The sizing of the equipment was proposed according to previous studies [5, 6, 39], while the ABE downstream process units were designed, employing shortcut methods and the sensitivity analysis tool available in the process simulator, followed by rigorous simulation.

The process flowsheet (see Fig. 3) starts feeding water (102) with sulfuric acid (103) to obtain a sulfuric acid

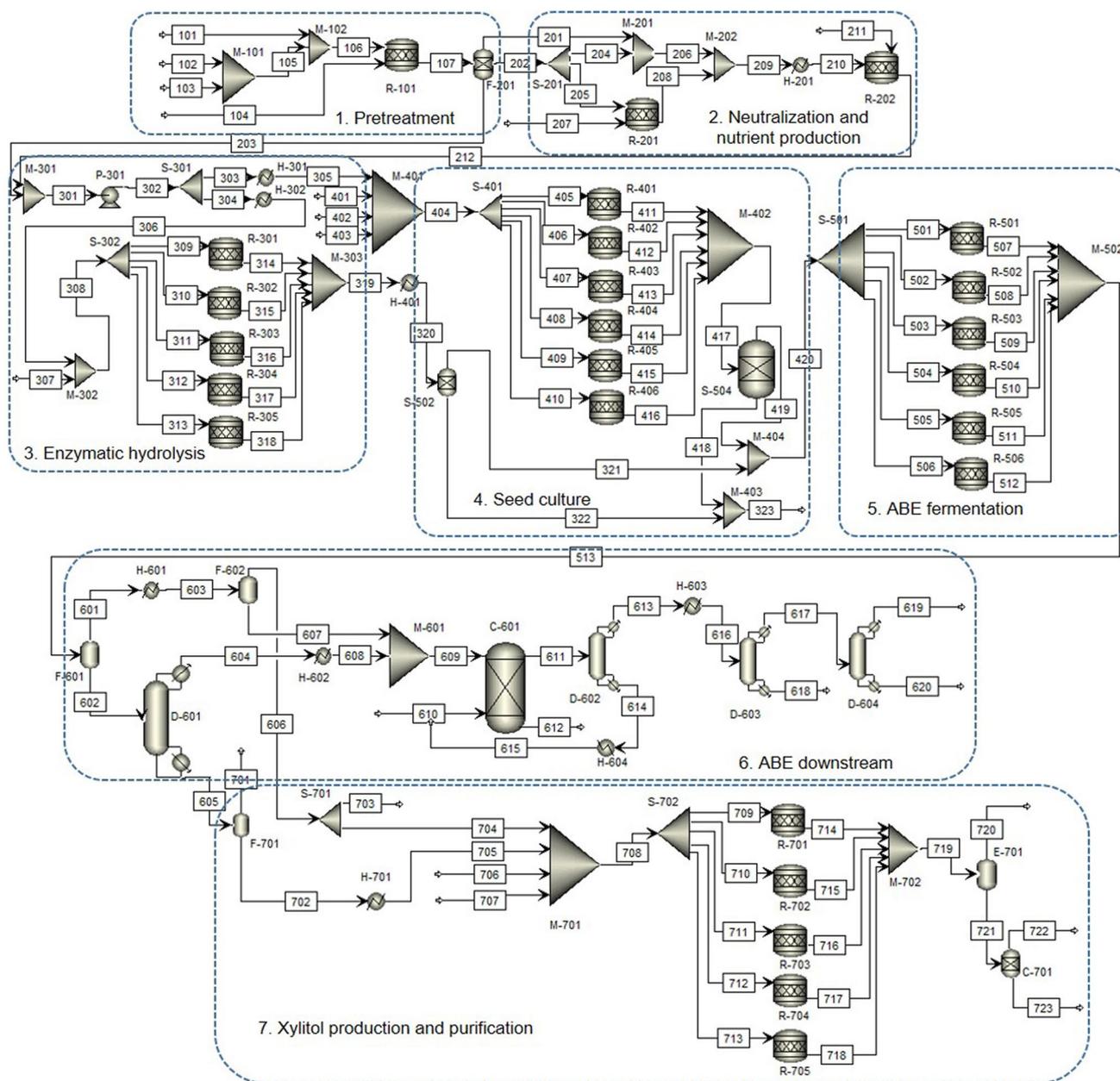


Fig. 3 Process flowsheet for the biorefinery: ABE and xylitol production

solution (6% wt/wt) in a mixer (M-101), then the sugarcane bagasse (101) is mixed with the sulfuric acid solution in a mixer (M-102). This mixture is fed to the continuous pretreatment reactor (R-101) where high pressure vapor (268 °C and 13 atm) is also fed (104), in order to reach the operation conditions of 120 °C in the reactor. The mass fraction of solids at the beginning of the chemical reaction was 30%.

The stream leaving the pretreatment reactor (R-101) is a vapor, solid and liquid mixture that is sent to a flash separator with an outstream for solids (F-201), where the solids leave the unit through stream 203 and the vapor and

liquid phases are separated in two streams (201 and 202, respectively). A portion of the liquid phase (3.11% of the total flowrate) is splitted (S-201) and fed to a continuous reactor (R-201), together with an ammonia stream (207) to produce ammonium sulfate, which is employed as a nitrogen source for microorganism growth and reproduction. The reaction at R-201 is carried out at 1 atm and 50 °C with a conversion of 89% for sulfuric acid. The stream leaving the reactor is mixed (M-202) with the liquid and vapor flowstreams, coming from a mixer (M-201). This mixture passes through a heat exchanger (H-201) to

Table 1 Design specification of main equipment

Process section	Equipment	Design specifications
Pretreatment	R-101	T = 120 °C; P = 12 atm; CC = 0.2765; HC = 0.57; CO
	F-201	T = 102 °C; P = 1 atm; CO
	Chemical reaction	$[C_6H_{10}O_5]_n + nH_2O \rightarrow nC_6H_{12}O_6$ at R-101
Neutralization and nutrient production	R-201	T = 50 °C; P = 1 atm; SAC = 0.89; CO
	H-201	T = 25 °C; P = 1 atm; CO
	R-202	T = 44 °C; P = 1 atm; SAC = 1; CO
	Chemical reactions	$2NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$ at R-201 $H_2SO_4 + 2NaOH \rightarrow 2H_2O + Na_2SO_4$ at R-202
Enzymatic hydrolysis	P-301	PI = 0.1 atm; CO
	H-301	T = 37 °C; P = 1.1 atm; CO
	H-302	T = 50 °C; P = 1.1 atm; CO
	R-301–R-305	T = 50 °C; P = 1 atm; CC = 0.66; RT = 36 h; VS = 904 m ³ (each); VN = 5; BO
	Chemical reaction	$[C_6H_{10}O_5]_n + nH_2O \rightarrow nC_6H_{12}O_6$ at R-301 – R-305
Seed culture	H-401	T = 37 °C; P = 1 atm; CO
	R-401–R-406	T = 37 °C; P = 1 atm; CC = 0.3; GC = 0.95; VS = 121 m ³ (each); VN = 6; RT = 36 h; BO
	S-502	Solid split factor = 1; outlet stream at the bottom
	S-504	Solid split factor = 1; outlet stream at the bottom
	Chemical reactions	$[C_6H_{10}O_5]_n + nH_2O \rightarrow nC_6H_{12}O_6$ at R-401 – R-406 $C_6H_{12}O_6 + 1.2NH_3 \rightarrow 6CH_{1.8}O_{0.5}N_{0.2} + 0.3O_2 + 2.4H_2O$ at R-401 – R-406
ABE Fermentation	R-501–R-506	T = 37 °C; P = 1 atm; CC = 0.897; RT = 48 h; VS = 1,203 m ³ (each); VN = 6; BO
	Chemical reaction	$18C_6H_{12}O_6 \rightarrow 6C_3H_6O + 12C_4H_{10}O + 2C_2H_5OH + 38CO_2 + 12H_2 + 12H_2O$ at R-501 – R-506
ABE-downstream	F-601	T = 37 °C; P = 1 atm; CO
	F-602	T = 15 °C; P = 1 atm; CO
	H-601	T = 15 °C; P = 1 atm; CO
	D-601	P = 1 atm; TT = 90.8 °C; BT = 100.1 °C; RR = 1; NS = 10; FS = 2; KC in SLP: water; PC; CO
	H-602	T = 35 °C; P = 1 atm; CO
	H-603	T = 35 °C; P = 1 atm; CO
	H-604	T = 37 °C; P = 1 atm; CO
	C-601	P = 1 atm; Adiabatic; key compounds: water (FLP) and hexyl acetate (SLP); FS(fermentation broth) = 1; FS(hexyl acetate) = 14; feeding mass ratio of 1:8.86 (fermentation broth:hexyl acetate); PS (FLP) = 14; PS (SLP) = 1
	D-602	P = 1 atm; TT = 106.1 °C; BT = 171.2 °C; RR = 2.6; NS = 37; FS = 27; KC in SLP: water; PC; CO
	D-603	P = 1 atm; TT = 69.2 °C; BT = 117.7 °C; RR = 2.13; NS = 37; FS = 14; KC in SLP: water; PC; CO
	D-604	P = 1 atm; TT = 54.1 °C; BT = 78.8 °C; RR = 8.38; NS = 37; FS = 14; KC in SLP: water; PC; CO
Xylitol production and purification	F-701	P = 1 atm; vapor fraction = 0.7; CO
	S-701	Split factor for H ₂ /CO ₂ = 0.92, T = 15 °C; P = 1 atm; CO
	H-701	T = 30 °C; P = 1 atm; CO
	R-701–R-705	T = 30 °C; P = 1 atm; XC = 0.79; GC = 1; RT = 15 h; VS = 147 m ³ (each); VN = 5; BO
	E-701	T = 100 °C; vapor fraction = 0.99; CO
	C-701	Split factor for xylitol = 1; outlet stream at the bottom
	Chemical reactions [42]	$100C_5H_{10}O_5 + 8.75O_2 + 7NH_3 + 37H_2 \rightarrow 86C_5H_{12}O_5 + 35CH_{1.8}O_{0.5}N_{0.2} + 35CO_2$ at R-701 – R-705 $C_6H_{12}O_6 + 3O_2 + 0.6NH_3 + 0.3H_2 \rightarrow 3CH_{1.8}O_{0.5}N_{0.2} + 3CO_2 + 4.5H_2O$ at R-701 – R-705

Table 1 (continued)

CC cellulose conversion, *HC* hemicellulose conversion, *SAC* sulfuric acid conversion, *GC* glucose conversion, *XC* xylose conversion, *CO* continuous operation, *BO* batch operation, *T* temperature, *P* pressure, *PI* pressure increase, *RT* reacting time, *TT* top temperature, *BT* bottom temperature, *RR* reflux ratio, *NS* number of stages, *FS* feed stage location, *VS* vessels size, *VN* vessels number, *KC* key compound, *FLP* first liquid phase, *SLP* second liquid phase, *PS* product stream, *PC* partial condenser

reach 25 °C and then is fed to a continuous neutralization tank (R-202), where it is mixed with the necessary sodium hydroxide (stream 211).

The neutralized liquid flowstream (212) and the solid stream (203) are mixed in the M-301 unit. The solid–liquid stream is divided in a splitter (S-301) in two streams, 10% of the flowrate (303) is sent to the inoculation section and the 90% is sent (stream 304) to the enzymatic hydrolysis section.

The stream 304 pass by a heat exchanger (H-302) to increase its temperature up to 50 °C, before entering to the enzymatic hydrolysis reactors. A diluted enzyme stream (307) is also fed to the batch enzymatic hydrolysis reactors (R-301 – R-305). The fed ratio for enzyme must be 20 mg of enzyme for 1 g of cellulose, and the dilution for the enzyme must be 30% in water. The conversion from cellulose to glucose was 66%. The leaving stream from the enzymatic hydrolysis must decrease the temperature until 37 °C in a heat exchanger (H-401), to reach the appropriate conditions for the fermentation section.

The flowstream (303) sent to the inoculation section must reach 37 °C of temperature passing through a heat exchanger (H-301), subsequently the stream is mixed (in M-401 unit) with one diluted enzyme stream, and sent to the batch inoculation reactors (R-401 – R-406) to liberate the glucose molecules from solids. A diluted enzyme stream is also fed to the batch inoculation reactors, with the same enzyme/cellulose ratio and dilution percentage (as at the enzymatic hydrolysis section). The liberated glucose is used at the seed culture reactors to grow the microorganism up.

The stream (419) from the batch inoculation reactors (R-401 – R-406) and the stream (320) leaving the H-401 are sent to solid–liquid separators (S-504 and S-502, respectively). The liquid phase streams from the separators are mixed (M-404), while the solid phase streams are mixed in the M-403 unit and sent for its combustion for power generation (323).

The mixture from stream 420 is divided and fed to batch fermenters (R-501 – R-506) where the glucose is transformed into acetone, butanol, ethanol, water, carbon dioxide and hydrogen by the microorganism action. The percent of glucose converted into products was 89.7%.

The ABE fermenters are followed by a flash unit (F-601), which separates the leaving stream from the fermenters (R-501 – R-506) that contains liquid and vapor phases, the vapor phase is sent to the second flash unit (F-602) to recover the acetone and butanol from the mixture in liquid phase, and take out most of the hydrogen and carbon dioxide

leaving the fermenter as vapor. The liquid phase from F-601 is fed to the first distillation column (D-601), that separates most of the water, glucose, and xylose at the bottom of the column. The top stream from the D-601 is mixed (at M-601 unit) with the recovered butanol and acetone from F-602, and sent to the liquid–liquid extraction unit (C-601), where an extracting compound (hexyl acetate) is fed (610) in a mass ratio of 1:8.86 (fermentation broth:extractant) [40]. The objective is to separate the ABE from water, and the stream without ABE leaves the unit at the bottom stream (612). The extractant, rich with the ABE mixture (611), is fed to the D-602 to recover and recycle the hexyl acetate, which is previously cooled to 37 °C in the H-604 and then it is sent to the C-601 unit. The ABE mixture is sent to the distillation column D-603, where the butanol is obtained at the bottom (618) with a purity of 99.5% wt/wt, and a recovery ratio (stream 618/stream 616) of 0.99. The following distillation column (D-604) was employed to separate the produced acetone obtaining a 95% wt/wt of purity (619) and mass recovery of 98% (considering streams 619/513), the bottom stream (620) contains some ethanol and water with a composition close to the azeotropic point (84% wt/wt and 16% wt/wt, respectively).

The stream (605) leaving at the bottom of the column D-601, is fed to one evaporator operating at 1 atm and 100 °C, with the main objective of evaporating 70% of the water present in the stream. The liquid phase is sent to the H-701 to reduce the temperature to 30 °C, and then the stream (705) is mixed with the recovered hydrogen in the F-602 unit and some necessary reactants and additives (706, 707) in the batch fermenters for xylitol production (R-701 – R-705). The batch fermentation reactors convert the xylose into xylitol and the glucose is employed for cell growth. The xylose and glucose conversion to products were of 79% and 100%, respectively.

The stream (719) leaving the fermentation reaction is sent to a vacuum unit (0.74 atm and 100 °C) to remove most of the water (almost 99%) in the top stream (720) and the stream with the xylitol is sent to the crystallization unit (C-701) for the final purification step to recover the xylitol (723).

Scheduling for Combining Batch and Continuous Operation

The process configuration combined the continuous and batch operation modes. In order to perform a reliable analysis of the process, it is necessary to propose an operation

scheduling, which must include the filling, reaction, drawing and idle that are repeated periodically. The scheduling was developed based on the size of the reactors, the flowrates of the process and the reacting time.

The Fig. 4 illustrates the fed-batch operation for the reactors of the enzymatic hydrolysis, seed culture, ABE (see Fig. 4a) and xylitol production sections (see Fig. 4b). The schedule depicted in Fig. 4a for enzymatic hydrolysis and seed (see left column) could be understood as follows: for reactor number one the periodic operation lasts 60 h. It starts with a loading (12 h), followed by a reaction time (36 h) and finally it ends with 12 h of drawing/emptying the content of the reactor. Once the first cycle is completed, the next cycle starts again by repeating the same schedule. The first fermentation reactor starts after 48 h then following for a similar schedule 12, 48 and 12 h. There is a variation in the reaction time for the fermentation section, because this operation requires of 12 extra hours to reach the desired product titers. In addition, it is necessary to add an extra fermentation unit (being 6 in total), to keep the same schedule.

As far as xylitol production is concerned, the reaction section also operates with 5 reactors, and follows a similar schedule but the filling, reaction and drawing period last 5, 15 and 5 h, respectively.

Economic Analysis of Process Configurations

There is a general idea about the not profitability of biofuels production and that the parallel production of value-added compounds could significantly improve the economics of the process. Thus, this work analyzed the sole ABE production, and the simultaneous production of ABE and xylitol in a biorefinery platform. The NPV, IRR and PBP were used to make the economic analysis. This study considered a desired return of investment (ROI) and interest rate of 20% per year, straight line depreciation method and 11 years for the economic life of the project.

The evaluation was done performing a sensitivity analysis relying on the commercial price for butanol (1.5–2 US\$ kg⁻¹) [43], acetone (1.16 US\$ kg⁻¹) [2] and xylitol (5–9 US\$ kg⁻¹) [43]. Table 2 shows the cost of the compounds used in the process and included in the calculations.

The sensitivity analysis was done considering: 1) only the selling price of butanol and 2) the combination of the prices for butanol and xylitol. Table 3 illustrates the economic indicators results with the variation of the butanol price (2.18–2.3 US\$ kg⁻¹). The case with the lower butanol price and positive financial indicators was for the butanol cost of 2.18 US\$ kg⁻¹ (B1); below that selling price, a negative indicator was obtained at the end period for the economic life of the project. The scenarios for butanol selling price higher than 2.30 US\$ kg⁻¹ (B4) were not evaluated,

since it is more expensive than current prices in the market of butanol produced from crude oil.

The sensitivity analysis for butanol and xylitol production started taking 2.18 US\$ kg⁻¹ for butanol price as base case and considering a range of xylitol prices in the market. The results show that it is possible to obtain a positive NPV, with different combinations of butanol and xylitol selling prices. The lowest selling price that can be obtained for butanol was 1.8 USD kg⁻¹ with 6 USD kg⁻¹ for xylitol (option BX1). The combination (BX2) for the lowest selling price of xylitol was 5 USD kg⁻¹ with 1.9 USD kg⁻¹ for butanol. Another combination (BX3) that could be considered is for the selling price of 1.9 and 6 USD kg⁻¹ for butanol and xylitol, respectively. The previous combinations are inside the range of the current selling prices for butanol and xylitol (1.5–2 and 5–9 USD kg⁻¹, respectively), therefore, the options BX1–BX3 are suitable to be set for obtaining revenues maintaining reasonable prices in the market, with the difference that the results of this work would obtain a renewable product. Whether the decision makers and stakeholders want to be in the butanol market with a competitive price, the best combination would be the selling prices for BX1, reducing 17% the butanol selling price whether it was compared with producing only ABE (B1). The option BX3 is other possibility if the butanol selling prices is increased by 0.1 USD kg⁻¹ that would increase the revenues 2.4 times compared with BX1, at the end period of the economic life of the project. The riskiest analyzed option would be BX5, which would have the higher butanol selling price with a good xylitol price, obtaining 3.8 times more revenues, at the end of the economic life of the project when compared with BX1. The previous scenarios show that it is possible to have combinations of selling prices similar to the products in the market.

The economic analysis of this study was based on the rigorous simulations including all the necessary equipment, additives and nutrients employed in the different sections of the process. It is imperative to highlight that diverse studies do not include the mentioned inclusions, for that reason usually can obtain lower PBP and selling prices in the product.

The analyzed scenarios allowed to confirm that industrial production of butanol from sugarcane bagasse is profitable. The economics of the process could be also improved whether xylitol production is added to the process.

In situ Energy Generation

After analyzing the mass balance of the process, it was possible to note that there was certain amount of solids that was not converted. Only the 57% of the fed solids were processed and the rest left the process (see stream 323 in Fig. 3). Some previous works [5, 44] have proposed to handle the residual solids to produce pellets, and then they can be subsequently combusted to produce energy, which is possible because

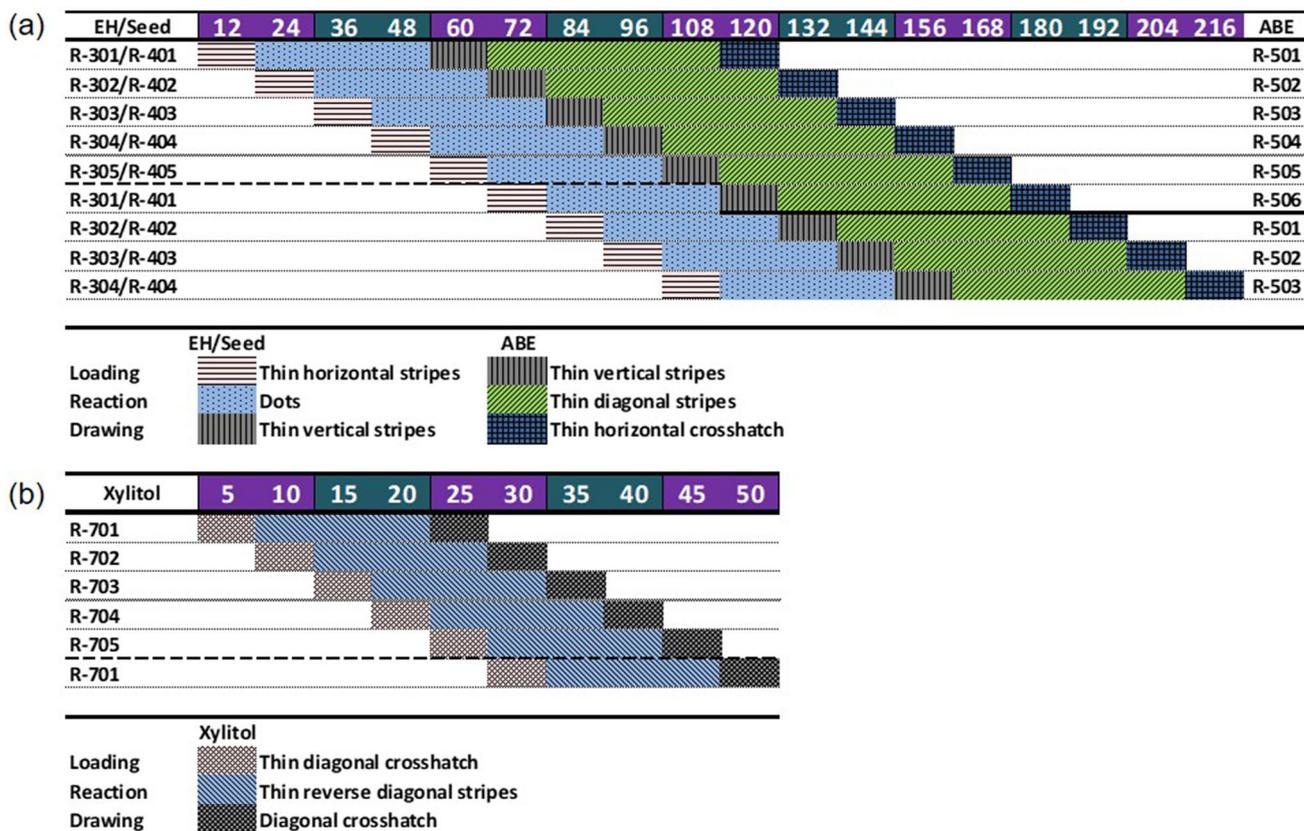


Fig. 4 Process scheduling for combining continues and batch scenarios at different sections of the process configuration: **a** enzymatic hydrolysis (EH), seed culture and ABE fermentation; **b** xylitol production

the residual solids have a relatively high heating value ($17.88 \text{ MJ kg-solid}^{-1}$) [45]. The flowrate of solids leaving the process was $12,434.69 \text{ kg h}^{-1}$, which could potentially produce $222,332.26 \text{ MJ h}^{-1}$ of energy. That amount of energy could be employed to produce vapor, instead of using diesel (around $5,214 \text{ kg h}^{-1}$). In addition, that would also mean some economic savings since the operating cost would be reduced by $6,441 \text{ US\$ h}^{-1}$, because diesel consumption would be reduced. The solid combustion would also have a positive impact to deplete around $15,426 \text{ kg h}^{-1}$ of carbon dioxide that would be produced by the diesel combustion. The use of residual solid material could help increasing the process sustainability.

General Discussion

There are still some issues to tackle, but this study allowed confirming that the simultaneous production of a biofuel and a value-added product could help to obtain a profitable process. Besides, the fact that a stream considered as waste can be used to produce xylitol allowed reducing the butanol cost, without sacrificing the financial revenues. Similar results were obtained previously [2] where biobutanol was

produced together with sugar and bioethanol in a first generation biorefinery.

However, as far as xylitol production in a biorefinery platform is concerned, Mountraki et al. [42] concluded that it is still necessary to enhance the biotechnological xylitol production, because the catalytic-based process is more profitable. Of course, there is still some room for developments since it could be possible to improve the performance in different sections of the process. For example, some studies have proposed that the xylitol production might be increased by proper model-based process design, and the operation of the batch reactor with optimal feeding policies [22], or the implementation of control strategies [46]. The computer-aided analysis has been already done and presented potential advances, but it is necessary to implement and combine those results in a pragmatic manner.

The butanol production could also be studied from the same modeling perspective, as xylitol production has been analyzed. In previous works [10, 47], the dynamic modeling for ABE process plant was already implemented, and that modeling platform also shows the possibility for analyzing some operating scenarios aiming to improve the ABE production. Obviously, it is important to recognize that

Table 2 Cost of the compounds employed to perform economic analysis

Category	Compound	Cost [US\$ kg ⁻¹]
Feedstock	Sugarcane bagasse ^[5, 7]	0.03
Additives	Sulfuric acid ^[43]	0.085
	Ammonia ^[43]	0.7
	Enzymes ^[5, 7]	1.85
	NaOH ^[43]	0.32
	KH ₂ PO ₄ ^[43]	0.10
	(NH ₄) ₂ HPO ₄ ^[43]	0.30
	MgSO ₄ ·7H ₂ O ^[43]	0.04
	CaCl ₂ ^[43]	0.12
	Myo-inositol ^[43]	1.00
	Calcium pantothenate ^[43]	1.00
	Thiamine-HCl ^[43]	1.00
	Pyridoxal-HCl ^[43]	1.00
	Biotin ^[43]	8.00
	FeCl ₃ ^[43]	0.05
	MnSO ₄ ·H ₂ O ^[43]	0.10
	ZnSO ₄ ·7H ₂ O ^[43]	0.24
CuSO ₄ ·5H ₂ O ^[43]	1.00	
Products	Butanol ^[43]	1.5 - 2
	Xylitol ^[43]	5 - 9
	Acetone ^[2]	1.16

Table 3 Results of the economic evaluation for ABE production and considering a biorefinery platform (ABE and xylitol production)

Product(s)	Option	Selling price, (US\$ kg ⁻¹)	NPV (MUS\$) at PBP moment	IRR (%)	PBP (years)	NPV (MUS\$) at the end period for economic life of the project
Butanol	B1	2.18	10.96	19.69	10.04	10.96
	B2	2.20	1.32	20.36	9.84	12.60
	B3	2.25	5.28	20.39	9.38	16.83
	B4	2.30	0.51	24.49	8.95	21.02
Butanol/Xylitol	BX1	1.80/6.00	5.96	21.17	10.81	5.96
	BX2	1.90/5.00	6.88	21.35	10.69	6.88
	BX3	1.90/6.00	1.59	22.77	9.83	14.2
	BX4	2.00/5.00	2.46	22.94	9.73	15.10
	BX5	2.00/6.00	9.37	24.34	9.03	22.43
	BX6	2.10/5.00	0.50	24.51	8.96	23.35

bioprocesses could be limited by the nature and the microorganism behavior. For instance, Mariano et al. [2], compared the butanol production evaluating the performance of a regular microorganism and a mutant strain, and they concluded that using the improved microorganism helps to be competitive in the butanol market.

Comparing to bioethanol research development, one interesting strategy has been done experimenting the combustion of wet ethanol [48] to reduce production cost, where López-Plaza et al. [48] evaluated the combustion of 80 vol% of wet ethanol, finding similar results when burning pure ethanol. In the proposed ABE process, the residual wet ethanol leaves the process (stream 619) with 85% wt/wt of ethanol, which might be considered as another potential biofuel because currently it is considered a waste due to the presence of water; other option is that could be used to produce energy in the production process.

Concluding Remarks

This work presents a significant finding since most of the time the feasibility of biofuel and high value-added products, have been highly criticized because of the energy use and economical drawbacks, such as the investment recovery. Therefore, this study has illustrated that it is possible to produce ABE and xylitol from sugarcane bagasse, with competitive market prices and positive economic indicators such as the NPV, IRR and PBP.

The sensitivity analysis in the economic evaluation allowed identifying that the production of one high value-added product, could significantly reduce the biofuel price. The production of xylitol was done with a waste stream, perhaps a further optimization analysis for the use of other waste streams could improve the economic results.

Moreover, the combustion of the solids residues in the process could potentially cover part of the energy necessary to produce the vapors in the plant, thereby, also having a positive impact in the environment, reducing significantly the carbon dioxide emissions from fossil sources.

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Compliance with Ethical Standards

Conflict of interest The authors declare no conflict of interest.

Human and Animal Rights This article does not contain any studies with human or animal subjects.

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