SIMULATION OF TREATMENT AND FERMENTATION STEPS FOR BIOETHANOL PRODUCTION

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ABSTRACT

In this work, a simulation of the production of wine was carried out in an autonomous distillery focused on the production of bioethanol from sugar cane. This bioproduct is produced from the fermentation of sugars present in this biomass. As a consequence, the following steps were carried out: definition of the components, thermodynamic model (NRTL) and main reactions involved; and process simulation. The simulated flowsheet in Aspen Plus software was organized into stages: sugarcane cleaning and milling; sugarcane juice treatment; sludge recycling; sugarcane juice concentration; and fermentation. From the simulated process, the main industrial steps involved in the treatment of sugarcane and the bioethanol production were known, obtaining wine in conditions similar to those found in Brazilian distilleries. In this context, the next stages of the work will involve the simulation of wine purification step, in order to meet current technical standards for hydrated fuel ethanol.

Keywords: Aspen Plus. Bioethanol. Fermentation. Simulation. Sugarcane.

1 INTRODUCTION

Ethanol is a colorless flammable liquid with a characteristic odor, with molecular formula C_2H_5OH and used in many industries. It is mainly produced from the fermentation of sugars present in biomass or lignocellulosic residues, which characterizes to be a biofuel known as bioethanol. The United States of America (USA) and Brazil are the main producers of bioethanol, using corn and sugar cane as raw materials, respectively. Due to its economic and environmental benefits, bioethanol is considered one of the most important biofuels in the world, being an interesting alternative to non-renewable fuels.[1]

From the pro-alcohol program created at the end of the 1970s, Brazil became a pioneer in the large-scale production and use of ethanol as a fuel. As a result, flex fuel vehicles were introduced into the Brazilian market, increasing the demand for ethanol fuel. For these reasons, Brazil is currently one of the largest producers and consumers of two products: anhydrous ethanol (AE), usually mixed to compose type C gasoline; and hydrated ethanol (HE), sold as fuel for internal combustion engines.[2]

As large-scale fuel bioethanol production in Brazil began approximately 50 years ago, improvements in the production process are required in order to remain competitive and reduce costs.[1] In this sense, the modeling and simulation steps in specialized software are excellent resources for integrating the production of bioethanol and bioproducts, based on biorefinery concepts, allowing to predict results without making changes in operation, optimize existing processes and suggest improvements in distillery designs.[3] Therefore, it is strategic to master computational tools such as the Aspen Plus simulator, aiming to simulate the conventional bioethanol production process.

In this context, the objective of this work was to simulate a wine production unit from sugarcane, in the Aspen Plus process simulator, as previous steps of bioethanol production. The main stages of the process were simulated, including sugarcane cleaning and milling; juice treatment and concentration; and fermentation. Finally, the conditions of the produced wine were compared to those found in Brazilian distilleries.

2 MATERIAL & METHODS

The simulation of the conventional wine production process from sugarcane was carried out in Aspen Plus simulator. In this sense, the main representative components of the process were selected.[4,5] The following criteria were adopted: to add the major components, including few binary interaction parameters for the thermodynamic model and prioritizing components found in the simulator databank.[3] Among the components defined for process simulation, the following stand out: water, phosphoric acid, calcium hydroxide, glucose (dextrose), sucrose, cellulose, silicon dioxide (impurity), potassium oxide (minerals), potassium chloride (salts), hemicellulose (d-xylose), calcium phosphate, lignin, aconitic acid (organic acid), calcium oxide (CaO), d-xylose, lignin, acetic acid, ammonia (NH_3), glycerol, hydrogen (H_2), sulfuric acid (H_2SO_4), yeast ($CH_{1.7}ON_{0.12}$), carbon dioxide (CO_2) and ethanol.[4,5]

For suitable representation of pure component properties, a property check was carried out for less usual components, using recognized articles and databases (NREL, Reaxys, PubChem and NIST chemistry webBook). The thermodynamic model chosen was the Non-Random Two-Liquid (NRTL), since offers advantages in modeling extremely non-ideal mixtures of highly polar components and partially miscible systems, offering a suitable representation of experimental phase equilibrium data. [4,5,6]

The reactions involved in the liming and fermentation stages involved in the wine production process from sugarcane were defined according to literature.[4] RSTOIC type reactors were used to simulate these steps, adopting conversions of 100% in liming, 100% in the inversion of sucrose to glucose, 90.5% of glucose to ethanol, 2.7% of glucose to acetic acid, 3.12 % of glucose to glycerol and 3.39% of glucose to yeast production (Saccharomyces cerevisiae).[4]

3 RESULTS & DISCUSSION

The flowsheet of the wine production process from sugarcane, simulated in Aspen Plus simulator, is shown in Figure 1, where the main stream results are presented in Table 1. The first step simulated was sugarcane cleaning, allowing removal of 70% of earth and other impurities through the SEP1 block. In the milling stage (SEP2), most of the lignocellulosic biomass was separated, including cellulose, hemicellulose and lignin, as well as small content of sugars. The sugarcane juice, free of impurities, was separated in SEP3 block, which represents industrial sieves and hydrocyclones.

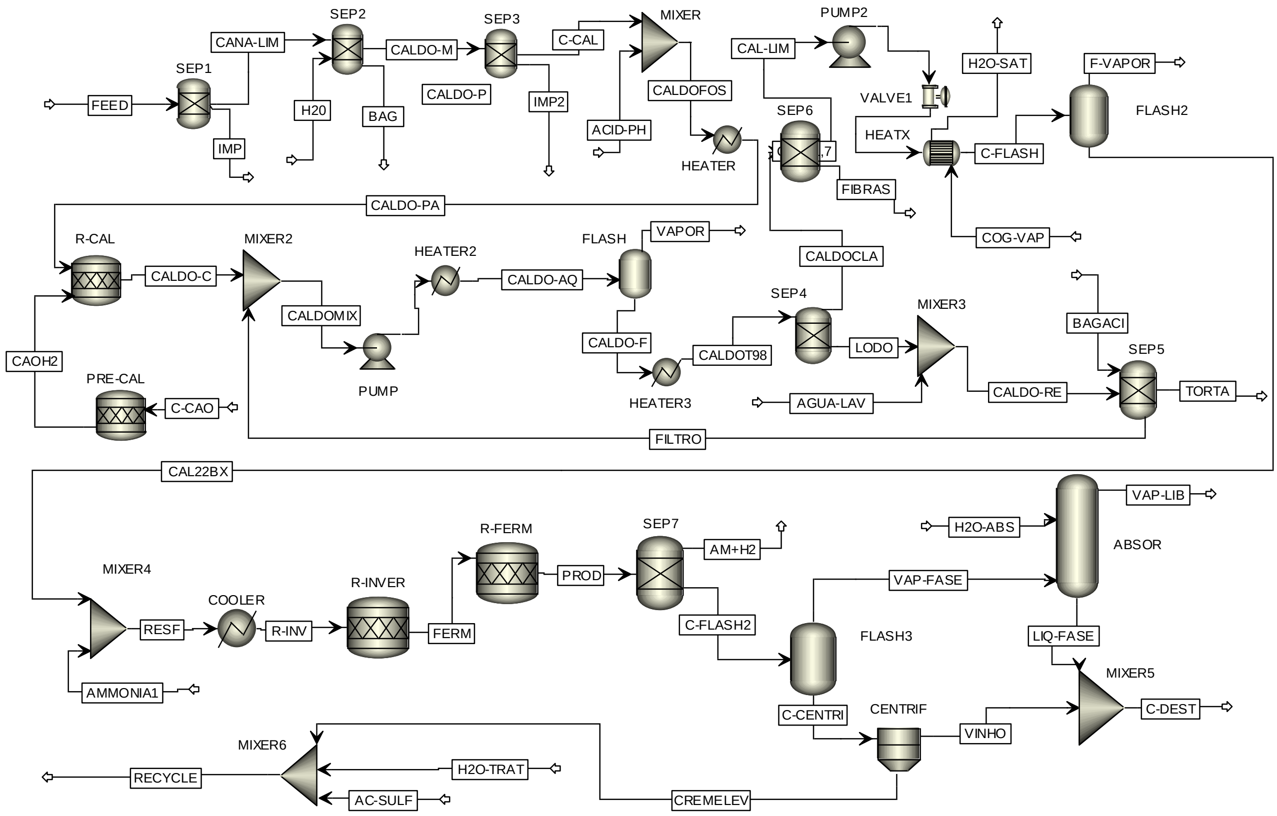

Figure 1 Flowsheet of the of the wine production process from sugar cane comprising the stages of sugarcane cleaning and milling, juice treatment and concentration, sludge recovery and fermentation.

Then, 85% phosphoric acid was added to the juice for liming using the MIXER block. This step promoted the sedimentation of impurities, allowing a greater concentration of the sludge to facilitate filtration. Liming step, which is the neutralization reaction of the juice to produce $Ca_3(PO4)_2$, took place in the RSTOIC reactor and produced the limed juice, which is mixed with the filter stream in the "MIXER2" block to produce the mixed broth. This broth was pumped at 2.5 bar and heated to 105°C for the treatment stage. In this process, the broth was heated in the "FLASH" block to evaporate part of the water and obtain the clarified broth with 15% Brix in the "SEP4" separator.

In the recycling stage, the sludge was treated to generate a filter stream, containing water and sugars, and the filter cake. The filter stream (FILTRO) was recycled and mixed to the juice in MIXER2 block. Next, the juice concentration step took place in FLASH2 block, where juice was concentrated into sugars (22°Brix). Then, the concentrated juice reacted in the R-INVER and R-FERM reactors, where sucrose was converted to glucose and glucose to ethanol and other by-products, respectively. After, the alcoholic product (PROD) was centrifuged to remove part of the yeast cream, producing the VINHO stream, which was mixed to the LIQ-FASE stream containing recovered sugars. As a result, the wine stream (C-DEST) was produced with an ethanol mass percentage of 10.86%, which is suitable to be injected into the distillation unit for hydrated ethanol production, since Brazilian distilleries generally obtain wine with 4°GL to 12°GL.[2]

Table 1 Stream results of the wine production process from sugar cane comprising the stages of sugarcane cleaning and milling, juice treatment and concentration, sludge recovery and fermentation.

Streams / Variables	FEED	BAG	CALDO-C	CALDO-F	CALDOCLA	TORTA	LODO
Temperature (°C)	25.0	25.0	70.0	100.4	98.0	25.0	98.0
Pressure (bar)	1.013	1.013	1.013	1.013	1.013	1.013	1.013
Mass flowrate (t/hr)	499.7	116.2	439.1	486.5	429.1	129616.3	57.4
Mass fraction							
Water	0.7200	0.5141	0.8133	0.8330	0.8500	0.0000	0.7057
Ca(OH)2	0.0000	0.0000	0.0088	0.0080	0.0000	0.0000	0.0676
Glucose	0.0060	0.0008	0.0066	0.0060	0.0067	0.0000	0.0005
Sucrose	0.1300	0.0168	0.1421	0.1270	0.1426	0.0000	0.0108
Cellulose	0.0500	0.1935	0.0011	0.0010	0.0003	0.4000	0.0061
Impurity (SiO2)	0.0060	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Minerals (K2O)	0.0050	0.0000	0.0057	0.0051	0.0000	0.0000	0.0435
Salts (KCl)	0.0070	0.0000	0.0080	0.0072	0.0000	0.1400	0.0609
Hemicellulose	0.0450	0.1742	0.0010	0.0006	0.0002	0.2200	0.0034
Ca3(PO4)2	0.0000	0.0000	0.0129	0.0116	0.0000	0.0000	0.0983
Lignin	0.0260	0.1006	0.0006	0.0005	0.0002	0.2400	0.0032
Organic acid	0.0050	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Streams / Variables	CAL22BX	FERM	PROD	C-FLASH	VAP-FASE	C-CENTRI	C-DEST
Temperature (°C)	115.7	34.0	34.0	34.0	34.0	34.0	34.3
Pressure (bar)	1.700	1.000	1.000	1.000	1.000	1.000	1.000
Mass flowrate (t/hr)	291	291	291	291	19	272	287
Mass fraction							
Water	0.7800	0.7685	0.7689	0.7690	0.0213	0.8217	0.8328
Ethanol	0.0000	0.0000	0.1069	0.1069	0.0256	0.1126	0.1086
Glucose	0.0099	0.2309	0.0007	0.0007	0.0000	0.0007	0.0007
Sucrose	0.2101	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Acetic acid	0.0000	0.0000	0.0042	0.0042	0.0000	0.0044	0.0042
NH_3	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
Glycerol	0.0000	0.0000	0.0074	0.0074	0.0000	0.0079	0.0075
H_2	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
H_2SO_4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Yeast	0.0000	0.0000	0.0062	0.0062	0.0000	0.0067	0.0000
CO_2	0.0000	0.0000	0.1057	0.1057	0.9531	0.0460	0.0461

4 CONCLUSION

From the simulated process, the main industrial steps involved in the treatment of sugarcane and the bioethanol production were known, obtaining wine in conditions similar to those found in Brazilian distilleries. In this context, the next stages of the work will involve the simulation of wine purification step, in order to meet current technical standards for hydrated fuel ethanol.

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