

Process Simulation of Ethanol Production from Jerusalem Artichoke Stalk

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ABSTRACT: *Lignocellulosic biomass can serve as raw material for ethanol production. However, lignocellulosic biomass is a complex mixture of carbohydrates that need additional processes for efficient ethanol production, such as pretreatment and hydrolysis before fermentation into ethanol. Therefore, this work mainly focused on the creation and simulation of a model of ethanol production from Jerusalem Artichoke Stalk (JAS) following experimental data and using the commercial software ASPEN Plus with and without a Heat Exchanger Network (HEN). Alkaline Hydrogen Peroxide (AHP) pretreatment was the first step for this process. The optimal conditions of AHP were a mixture of 2% w/w sodium hydroxide (NaOH) and 4% v/v hydrogen peroxide (H₂O₂) at 10% (w/v) solid-liquid ratio and 121°C for 90 min. After treatment, 10% AHP-JAS loading was fed to enzymatic hydrolysis at 50°C and the fermentation process at 30°C. The simulation suggested that a feedstock of 60,000 kg of JAS could yield 3,482.16 kg ethanol. The purification section by the extractive distillation system had 12 stages, a distillate to feed mole ratio (D/F) of 0.13, and a reflux mole ratio (R/R) of 1.5. The purity of the ethanol product was higher than 97 wt%. After the model simulation, HEN was designed by using Aspen Energy Analyzer. After the installation of HEN in this process, the ethanol plant with HEN showed a better result, which at 16.24 percentages reduced total cost compared to the process without HEN.*

KEYWORDS: *Lignocellulosic biomass, Jerusalem artichoke stalk, Ethanol production simulation, Alkaline hydrogen peroxide pretreatment, Aspen plus.*

INTRODUCTION

The problem of global warming is an issue of global significance. This problem is caused by many factors,

such as the release of carbon dioxide from vehicle engines and industrial operations. The use of renewable biofuels

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and clean energy sources had the potential to reduce global warming. Potential renewable energy sources include bioethanol, biodiesel, and biohydrogen produced from biomass [1-3]. Bioethanol is commercially produced by sugar fermentation from starch- and sugar-based feedstock such as corn, cassava, and sugarcane [4]. But these raw materials are important human foods and are expensive.

Lignocellulosic biomass feedstock does not compete with food use. Jerusalem Artichoke Stalk (JAS) is potential lignocellulosic biomass for producing energy in a biorefinery because of its traits such as resistance to environmental stresses and high biomass yield in suitable environments [5]. The stalk is the dominant biomass of Jerusalem artichoke. Jerusalem artichoke stalk comprises cellulose and hemicellulose that can be converted to sugar to produce ethanol. Also, inulin in the Jerusalem Artichoke Tuber (JAT) can be used to produce ethanol using inulinase-producing yeasts such as *Kluyveromyces marxianus* CBS1555 [5]. A suitable treatment for removing lignin and hemicellulose in JAS involves the use of dilute (0.5 % (v/v)) sulfuric acid followed by 1 M NaOH to hydrolyze the cellulose to fermentable sugars [6-7].

Aspen technology is well for simulation of chemical engineering processes and Heat Exchanger Networks (HEN) to develop processes with a reduced cost of operation [8]. Bioethanol production from lignocellulosic biomass involves pretreatment, hydrolysis, fermentation, and purification [9]. Pretreatment is the first step of lignocellulose bioconversion, which aims to deconstruct the recalcitrant structure of the feedstock and separate the major components of cellulose, hemicelluloses and lignin so that the cellulose could be more efficiently hydrolyzes to fermentable sugars. Among various pretreatment technologies, Alkaline Hydrogen Peroxide (AHP) pretreatment is efficient in increasing the accessibility of cellulose for subsequent bioconversion by enzymes or microorganisms to sugars [10-11].

The enzymatic hydrolysis is used to convert cellulose from the pretreated JAS to glucose for microbial fermentation. The glucose is then fermented to ethanol using the yeast *Saccharomyces cerevisiae* (*S. cerevisiae*) has been widely used in the industrial production of bioethanol [12]. When enzymatic hydrolysis and fermentation are performed sequentially, it is referred to as Separate Hydrolysis and Fermentation (SHF). Carbon dioxide (CO₂) is

a by-product of fermentation [13]. After fermentation, the broth is sent to a distillation unit to recover the ethanol with the desired specifications [14]. In the purification section, the aim is to achieve an ethanol concentration of more than 90%. Extractive distillation is most commonly used. Extractive distillation uses an added solvent to break the azeotrope mixture (95.63% ethanol and 4.37% water by weight) in the distillation column. The solvents should have low volatility. The solvents that are widely used are ethylene glycol and glycerol. *Gil et al.* [15] studied ethanol extractive distillation with mixed glycerol as a separating agent. In this work, the thermodynamic model was NRTL and a process was simulated using two extractive distillation columns (Radfrac), and solvent recovery. A solvent mixture of ethylene glycol and glycerol was used. The authors concluded that the solvent (60:40 mole ratio of ethylene glycol to glycerol) should be fed in the 4th stage of the extractive column.

In the present study, experimental data from the pilot plant and laboratories of Shanghai Jiao Tong University [16] were used to design a bioethanol production process from JAS. An integrated ethanol plant, including pretreatment, Separate Hydrolysis, Fermentation (SHF), and purification was simulated along with the specific operations, by using the commercial software Aspen Plus. Afterward, the simulated plant was analyzed for installation for a Heat Exchanger Network (HEN) to reduce cost. The HEN analysis used the Aspen Energy Analyzer.

EXPERIMENTAL SECTION

Feedstock, strain, and culture medium

Naturally dried JAS was milled to a size range of 1–10 mm and rinsed with water to remove dust and other impurities and then dried at 50 °C for 48 h in an oven. Cellic[®] Ctec2 (Novozymes, Bagsvaerd, Denmark), a commercial enzyme, was purchased. The *S. cerevisiae* SPSC01 developed at the authors' laboratory and deposited at China General Microbiological Culture Collection Center (CGMCC) was employed in this work. The YPD medium for seed culture consisted of glucose 30 g/L, yeast extract 4 g/L, and peptone 3 g/L.

Experimental description

The experiments of ethanol production in the laboratory comprised two parts, the AHP pretreatment, and SHF. AHP pretreatment was used to pretreat the JAS biomass before SHF. The above prepared JAS was pretreated

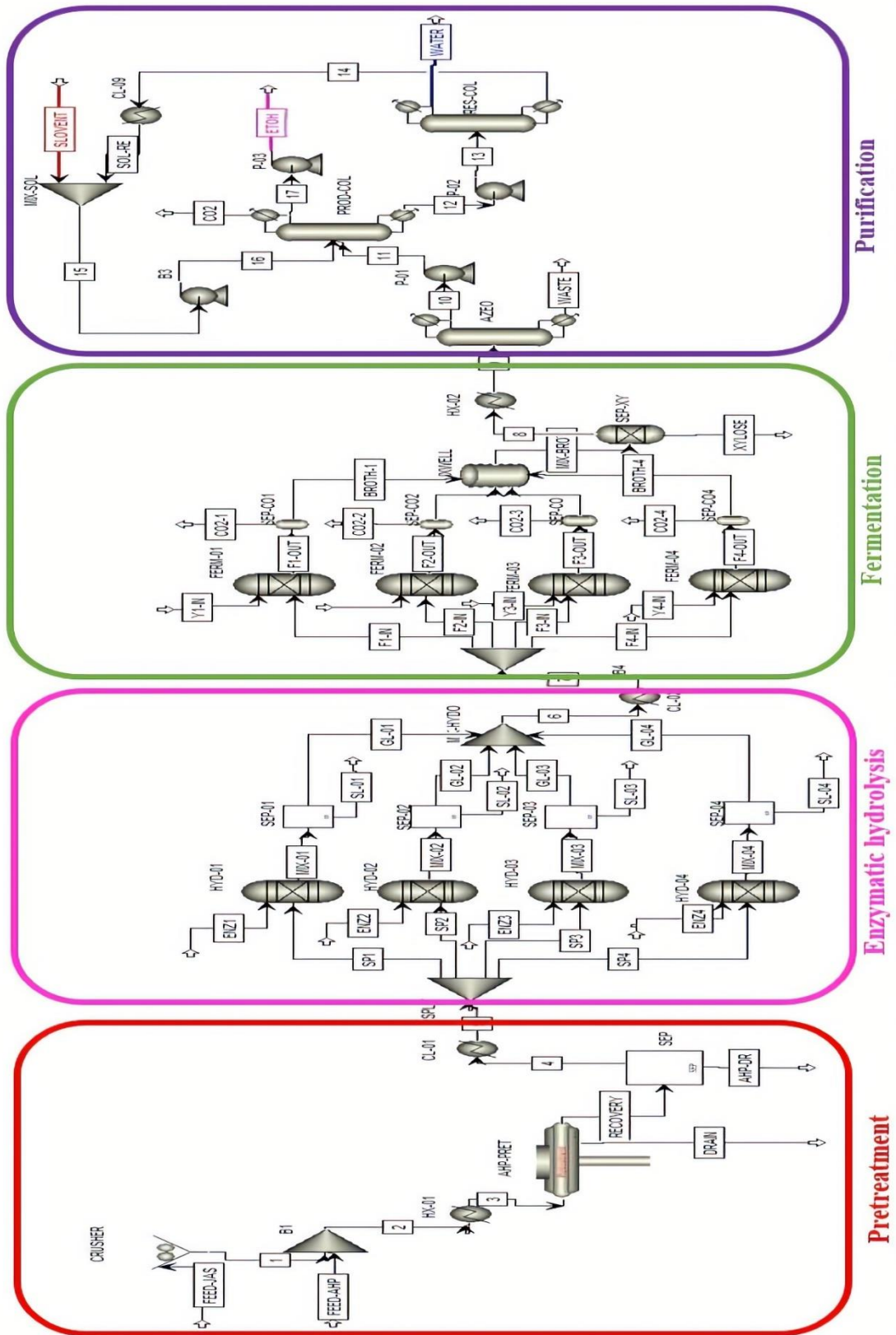


Fig. 1: Ethanol process flowsheet in Aspen Plus.

by a mixture of NaOH (1, 2, or 3 %, w/w) and H₂O₂ (2, 3 or 4 %, v/v) at 10% (w/v) solid-liquid ratio and 121 °C for 90 min. The treated JAS was washed to neutral pH by water and dried at 45 °C for 48 h in an oven.

Next, the treated JAS was used in SHF. SHF consisted of enzymatic hydrolysis and fermentation by yeast. For enzymatic hydrolysis pretreated JAS solids, 10 g dry AHP-JAS (pretreated JAS) was enzymatically hydrolyzed in a 100 mL of 0.05 M sodium citrate (pH 4.8) buffer containing the Cellic[®] Ctec2 at a loading 20 FPU/g substrate (20 filter paper units of enzymes per 1g of AHP-JAS) at 50 °C. For ethanol fermentation, the self-flocculating yeast *S. cerevisiae* SPSC01 with a 10% (v/v) inoculation level was used at 30 °C and 150 rpm stirring rate.

Heat Exchanger Network (HEN)

A Heat Exchanger Network (HEN) is used in industrial processes by depicting the interaction between process streams and utilities to meet the plant requirement and can be designed efficiently using process integration. HEN was used to reduce cost and energy. HEN was analyzed using Aspen Energy Analyzer.

Physical property method

The physical property method is a set of equations to predict the properties of the chemical system in the process. The complete plant was simulated using Aspen Plus V8.8. The simulation utilized NRTL (Non-Random Two liquids) with Henry's Law for the thermodynamic method because ethanol and water have an azeotropic behavior.

Process simulation

The complete flowsheet of ethanol production from JAS is shown in Fig. 1. This flowsheet was used to design and simulate ethanol production based on experimental information. The process was designed to use 60000 kg/day of the JAS feedstock.

Firstly, JAS biomass (Feed-JAS) with the initial content of 35.93% cellulose, 22.21% hemicellulose, 17.26% lignin, and 2.31% ash, was fed to a multiple roller crusher (CRUSHER) in which the particle size could be reduced to a range of 1–10 mm before the pretreatment. The pretreatment unit (AHP-PRET) was formulated using mathematical models in Aspen Custom Modeler (ACM) before porting to ASPEN Plus. The pretreated JAS, or AHP-JAS (Recovery), was fed to the enzymatic hydrolysis

units (HYD-01,02,03,04) in parallel to convert cellulose and hemicellulose to simple glucose and xylose by using the cellulase enzyme (Enz1,2,3,4). The enzymatic hydrolysis unit operated at 50 °C. After pretreatment and enzymatic hydrolysis, the sugar stream (GL-01,02,03,04) was fed to the fermentation unit (FERM-01,02,03,04) for fermentation to ethanol (BROTH-1,2,3,4). Carbon dioxide (CO₂-1, CO₂-2, CO₂-3, and CO₂-4) was a by-product during fermentation and vented out of the system in the unit (SEP-CO1, CO₂, CO₂, CO₂, CO₃).

The fermentation broth containing mostly ethanol, xylose, and water was sent to the storage tank (MIXWELL). Xylose, a by-product, was separated before the broth was fed to the next unit. This broth (8) contained residual ethanol and water because ethanol could not be recovered to a purity of higher than 97% as a consequence of azeotropy. Therefore, the extractive distillation technique (PROD-COL) was used to achieve the product specification, and ethylene glycol (Solvent) was used for breaking the azeotrope. Ethanol at the top had a purity of 97 wt%, while the water and solvent from the bottom of the column were processed in the solvent recovery column (RES-COL). Some makeup solvent was required.

RESULTS AND DISCUSSION

Pretreatment

The AHP experimental information obtained from the laboratory is shown in Table 1. The optimal condition used for AHP pretreatment assured suitable cellulose content. The response surface technique was used on data from nine experiments to identify the optimal conditions for AHP pretreatment. The identified optimal AHP pretreatment as requiring 2% NaOH and 4% H₂O₂.

The models for the content of cellulose, hemicellulose, lignin, ash, and total pretreated JAS biomass solids for various concentrations of NaOH (% w/w) and H₂O₂ (% v/v) used in pretreatments, are shown in Table 2. These model equations were obtained by analysis of the experimental data by Minitab software.

The results were for a total flow rate of raw JAS of 2,500 kg/h. The composition of the JAS is summarized in Table 3. The result shows that 36.44% of the material was removed from raw JAS during the AHP process, the cellulose increased to 49.80 from 35.93% dry solid weight, while the hemicelluloses and lignin were decreased to 13.33% from 22.21% and 7.03% from 17.26% dry solid weight, respectively.

Table 1: The composition of JAS after AHP pretreatment.

Concentration (%)		Biomass recovery*	Composition (dry wt%)			
NaOH	H ₂ O ₂		Cellulose	Hemicelluloses	Lignin	Ash
0	0	100	35.93	22.21	17.26	2.31
1	2	74.25	39.15	15.52	9.78	5.00
1	3	75.75	41.76	14.86	8.08	7.20
1	4	73.00	42.41	14.54	10.60	6.40
2	2	68.25	45.65	13.46	11.78	1.90
2	3	64.00	49.59	13.27	7.14	1.40
2	4	62.50	50.37	13.33	7.10	2.03
3	2	61.25	50.89	12.14	6.05	1.09
3	3	60.75	49.72	11.89	5.90	0.97
3	4	61.50	50.50	12.52	5.94	1.03

* Biomass recovery was defined as the ratio of pretreated biomass to raw biomass.

Table 2: The modeling equation of JAS after AHP pretreatment.

Composition	Modeling equation	R ²
Cellulose	$11.12+19.72\times N+8.00\times H-0.91\times N\times H-3.09\times N^2-0.82H^2$ (1)	0.96
Hemicellulose	$21.11-3.18\times N-2.07\times H+0.34\times N\times H+0.19\times N^2+0.21H^2$ (2)	1.00
Lignin	$13.27-1.76\times N-0.68\times H$ (3)	0.53
Ash	$2.438-7.37\times N+6.31\times H-0.557\times N\times H+1.625\times N^2-0.814\times H^2$ (4)	0.94
Biomass Recovery	$99.12-20.60\times N-3.97\times H+0.38\times N\times H+3.22\times N^2+0.35H^2$ (5)	0.95

N = NaOH concentration of between 1 – 3 (%w/w)

H = H₂O₂ concentration of between 2 – 4 (% v/v)

Separate Hydrolysis and Fermentation (SHF)

The SHF part consisted of two-unit operations (enzymatic hydrolysis and fermentation units) that were modeled a yield reactor (HYD-01,02,03,04 and FERM-01,02,03,04, respectively) in Aspen Plus. Firstly, enzymatic hydrolysis units used the glucose yield based on the cellulose from AHP-JAS was 0.5144 g/g and converted to ethanol, while xylose yield based on the hemicellulose from AHP-JAS was 0.5144 g/g from experimental data. Then, fermentation units used the ethanol yield based on

the glucose was 0.461 from experimental data, while xylose assumed can't convert to ethanol.

For the mass flow was the AHP-JAS (RECOVERY) at various enzyme loadings (ENZ1,2,3,4) and operated at a temperature of 50°C. After the enzymatic hydrolysis unit, the mass flow was the hydrolysate (7) fermented at various yeast loadings (Y1, Y2, Y3, Y4-IN), and operated at a temperature of 30°C. The results were for a total flow rate of raw JAS of 2,500 kg/h. The composition of ethanol production is summarized in Table 4.

Table 3: The composition of AHP-JAS pretreatment

Concentration		Stream			
		Feed-JAS	Feed-AHP	Drain	Recovery
Mass Flow kg/hr					
Cellulose		898.25	0	138.84	659.41
Hemicellulose		555.25	0	279.01	176.24
Lignin		431.50	0	238.41	93.09
Water		0	7833.02	0	7833.02
Ash		57.75	0	31.82	25.93
Other		557.25	0	222.92	369.45
Sodium hydroxide		0	166.66	166.66	0
Hydrogen peroxide		0	333.32	333.32	0
Mass Frac					
Cellulose		0.359	0	0.015	0.498
Hemicellulose		0.222	0	0.030	0.133
Lignin		0.173	0	0.026	0.070
Water		0	0.940	0.847	0
Ash		0.023	0	0.003	0.020
Other		0.223	0	0.024	0.279
Sodium hydroxide		0	0.020	0.018	0
Hydrogen peroxide		0	0.040	0.036	0
Total Flow	kg/h	2500.00	8333.00	9244.00	1589.00

After AHP pretreatment, the cellulose and hemicellulose (4) solids were fed to the enzyme reactor at 791.32 and 211.49 kg/h, respectively. The enzyme hydrolyzed both cellulose and hemicellulose to produce glucose and xylose. Glucose and xylose production rates were 411.72 and 108.96 kg/h, respectively. Then glucose and xylose were sent to the fermenter to produce ethanol.

Fermenter produced ethanol at a rate of 189.80 kg/h. The vapor from the fermenter had a flow rate of about 221.91 kg/h. This vapor mostly contained CO₂ and was vented out of the system. The fermentation broth was sent to the purification section to purify the product.

Overall mass balance

Biomass loss with a single step is inevitable, thus an overall mass balance is necessary to evaluate the integrated process. As shown in Fig. 2 developed from the laboratory data in Table 1 and 4 at 10% AHP-JAS (pretreated JAS), although 36.44% biomass was removed from raw JAS during the AHP process at a mixture of 2% NaOH and 4% H₂O₂, cellulose loss was much lower, and its recovery was as high as 88.10% (31.65 from 35.03%), while the mass recovery of hemicelluloses and lignin were only 38.09% and 25.89%, respectively. For the SHF process, 51.44%

Table 4: The composition of ethanol production.

Concentration		Stream		
		Recovery	GL-01,02,03,04	BROTH-1,2,3,4
Mass Flow kg/hr				
Cellulose		791.32		
Hemicellulose		211.49		
Lignin		111.71		
Ash		31.11		
Other		443.36		
Glucose		0	411.72	
Xylose		0	108.96	108.96
Ethanol		0		189.80
CO ₂				221.91
Mass Frac				
Cellulose		0.498		
Hemicellulose		0.133		
Lignin		0.070		
Other		0.279		
Glucose		0	0.791	
Xylose		0	0.209	0.209
Ethanol		0		0.365
CO ₂				0.426
Total Flow	kg/h	1589.00	520.67	520.67

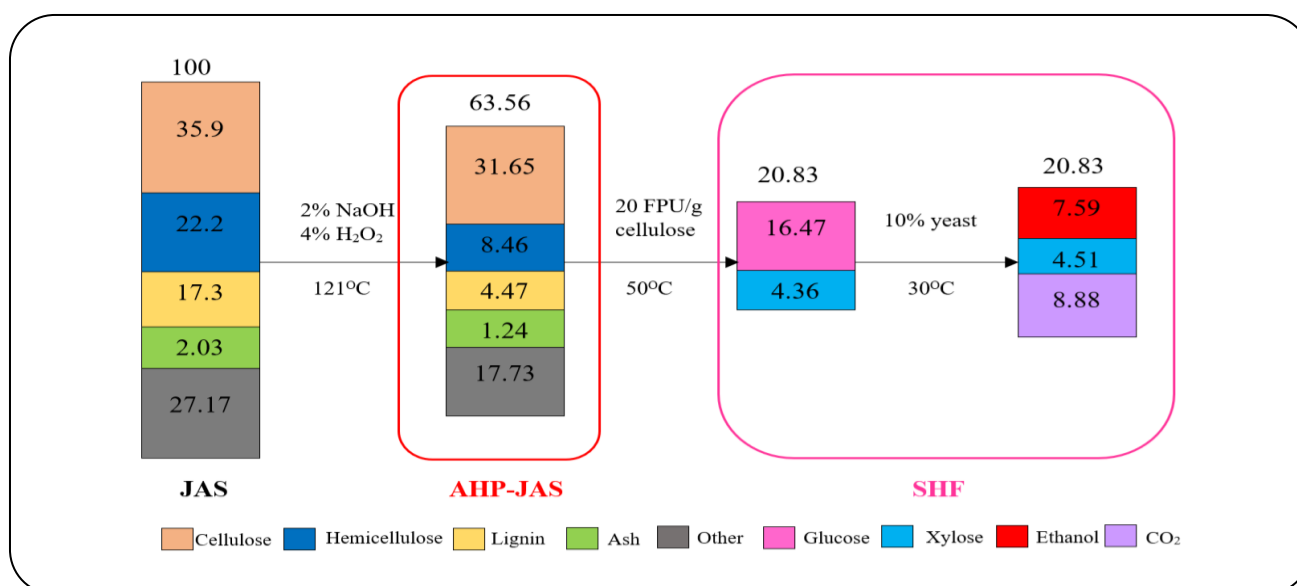


Fig. 2: Diagram for overall mass balance base on 100 g of JAS. The mass unit is gram (g).

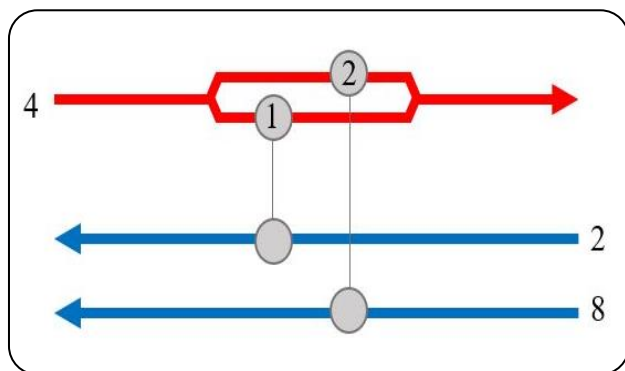


Fig. 3. Grid diagram of heat exchanger network

glucose was released from AHP-JAS and converted to ethanol, and ethanol yield based on the total sugar was 0.461 g/g.

Purification

The carbon dioxide streams (CO₂-01,02,03,04) were a by-product of fermentation and were vented out of the system (Sep-CO1, CO₂, CO₃, CO₄). The fermentation broth (9) mostly contained ethanol and water. This mixture could not be purified to more than 97% ethanol because of azeotropy. Therefore, extractive distillation (PROD-COL) was used to achieve the required product specification, and ethylene glycol (Solvent) was used for breaking the azeotrope. Ethanol at the top had a purity at 97 wt% while the water and solvent from the bottom of the column were returned to a solvent recovery column (RES-COL) with some makeup solvent added.

In the purification section, the fermentation broth (10) was fed to the AZEO unit at stage 10 and passed through the extractive distillation column (PROD-COL). The feed-stage of the mixture (stream-11) is at 8 and the solvent (16) was fed at stage 4. The extractive distillation column (PROD-COL) had 12 stages. The distillate to feed mole ratio (D/F) was 0.13, and the reflux mole ratio (R/R) was 1.5. This column produced ethanol with a purity of more than 97 wt% (145.09 kg/h).

Heat exchanger network design

The complete flowsheet of ethanol production from JAS without the HEN had a total cost of energy 1.54×10^6 units/year or 115.13% of the target. Thus, a HEN was implemented to improve the efficiency of the process.

The process had one hot stream (4) and two cold streams (streams 2 and 8). The HEN was designed based

on pinch technology. Pinch methodology was used to find the optimum energy integration. The aim was to match hot and cold streams in the process to minimize the need for externally supplied utilities. The HEN was analyzed by using Aspen Energy Analyzer. This program analyzed the heat integration between hot and cold process streams without any external utility, as shown in Fig. 3.

After the installation of HEN in the process (Fig. 4), the total cost of energy was 4.59×10^5 units/year or 98.89% of the target. The ethanol plant with HEN showed a better result in which the total cost was reduced by 16.24% compared to the ethanol plant without the HEN.

CONCLUSIONS

Aspen Tech software was used for the simulation and Heat Exchange Network (HEN) design of a process for producing ethanol from lignocellulosic biomass of Jerusalem Artichoke Stalk (JAS). Experimental data contributed by the Shanghai Jiao Tong University laboratory were used for simulation and design. The pretreatment model was created in Aspen Custom Modeler (ACM). The optimal conditions of JAS pretreatment were a 10% (w/v) solid-liquid ratio in a medium containing 2% NaOH and 4% H₂O₂ at 121 °C for 90 min. The train of hydrolysis and fermentation (SHF section) was divided into four parallel sets to feed the continuous distillation section. The SHF process was modeled using a yield reactor in Aspen Plus. Based on the simulation 60,000 kg of JAS can provide 3,482.16 kg of ethanol. Purification by extractive distillation could achieve an ethanol purity of more than 97 wt%. Ethylene glycerol was the solvent for breaking ethanol-water azeotrope. The number of stages in this distillation column was 12, the distillate to feed mole ratio was 0.13, and the reflux mole ratio was 1.5. Implementation of a heat exchanger network resulted in a 16.24 percentage energy saving compared to an ethanol plant without the HEN.

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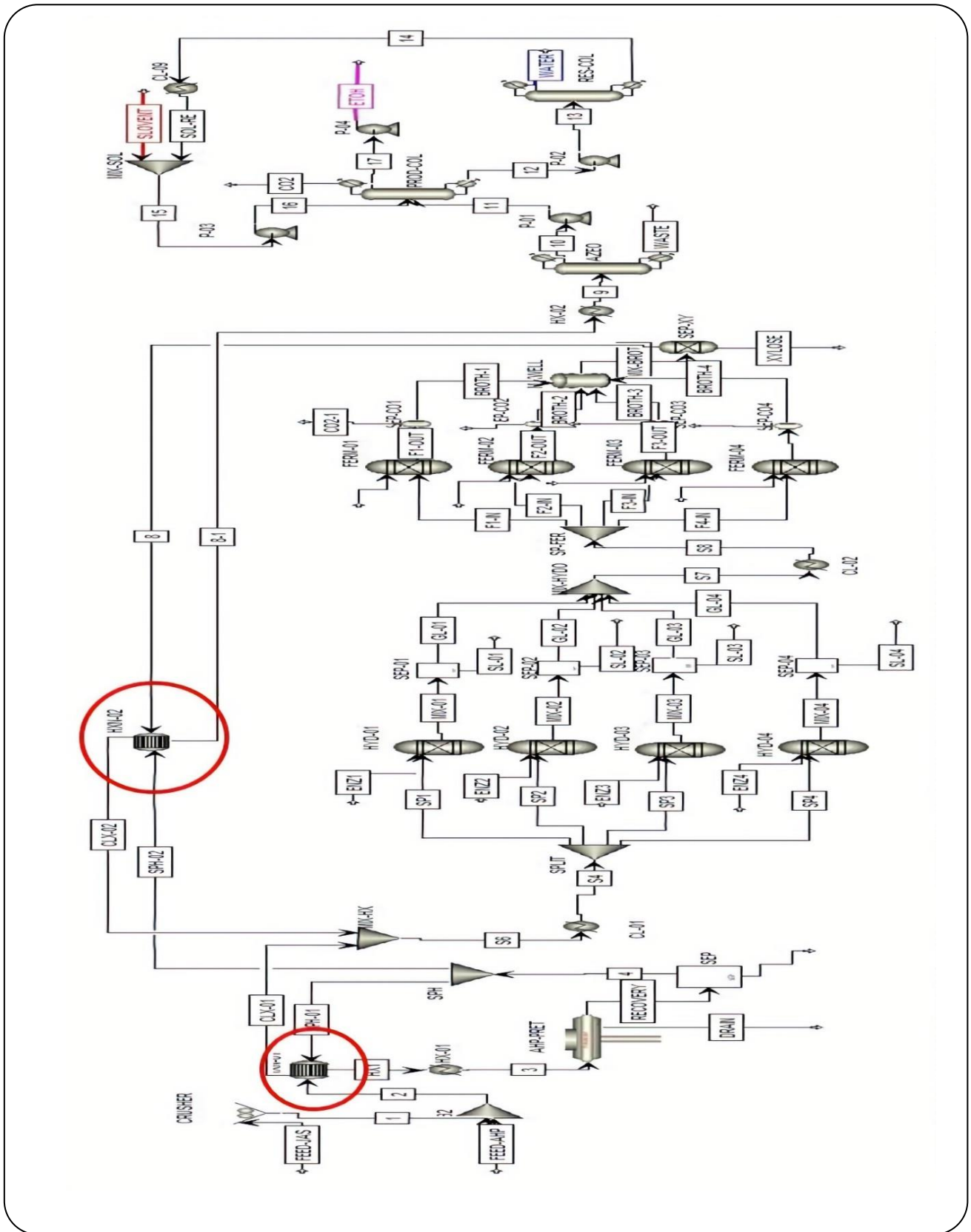


Fig. 4: Ethanol process with heat exchanger network.

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