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Computer-Aided Environmental Assessment and

Energy Integration of Bioethanol Production from

Rice Residues

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Abstract

In this paper, environmental assessment and energy integration of a bioethanol production plant from rice chaff is made. The main product of the plant is the bioethanol, which is one of the most used biofuel in the energy sector. The bioethanol production was simulated using ASPEN PLUS software, obtaining in this way a base case of study. Then, pinch analysis was used to benchmark the potential energy integration. To attain the energy targets, a heat exchange network was proposed to reduce both the heating and cooling utilities. Finally, an environmental analysis of both the base case and the integrated process was made using graphical user interface (GUI) tool WAR (WAste Reduction algorithm of the National Renewable Energy Laboratory - NREL), to determine the potential environmental impacts of the process and to perform an evaluation between the base case and the integrated one.

Keywords: Bioethanol, energy integration, rice, agricultural wastes, environmental assessment

1. Introduction

Due to energy crisis that is currently facing the society, one of the alternatives to mitigate the impacts of global energy demand is the biofuels production. These substances comes from biomass sources and have an interesting energy potential primarily because of the low cost of raw material [7]. According to an estimation reported in the literature [4], North region of Colombia had the potential to produce around 125.250 tons of rice that represents 319.888 tons of wastes.

The operation of the plant and the processes for bioethanol production demands a large energy supply, therefore it is common that operations costs of the process are very high. Energy integration methodology helps to reduce the industrial services of cooling and heating in order to mitigate the impact of the process in the availability of energy sources. This methodology involves the benchmarking of minimum requirements of industrial services via pinch analysis. The potential reduction is achieved by means of the design of a heat exchange network [2]. Also, environmental assessment methodology is used to determine the potentials impacts in several categories such as human toxicity for ingestion, aquatic toxicity, ozone depletion, among others [1].

2. Case Study: Bioethanol Simulation

The operation conditions of the bioethanol plant were stablished by reviewing the scientific literature. ASPEN PLUS software database does not have information about some substances that are involved in the operation of the plant. Therefore, these molecules were created using the data reported by the NREL, which allowed us to obtain simulation data very close to real conditions [9].

The simulated plant starts with the pretreatment process, which is carried out at 190°C, 19 atm, and diluted sulfuric acid as catalyst [6]. The operation continues with the cooling and subsequent neutralization of sulfuric acid used in the pretreatment reactor; this reaction use lime to balance the pH of the system. The plant was simulated applying a Simultaneous Saccharification and Co-fermentation (SSCF); the reactions in the bioreactor were taken from [10]:

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Celullose + H_2O \rightarrow Glucose
Glucose \rightarrow 2 Ethanol + CO_2
3 Xilose \rightarrow 5 Ethanol + 5 CO_2
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The products coming out of the reactor have low concentration of bioethanol, a notorious amount of water, and others substances that must be separated from the process. The purification of the ethanol is performed in a separation train where carbon dioxide is separated from the fermentation juice [6]. The stream passes to a second distillation tower, where azeotropic ethanol is obtained. Finally, the ethanol is purified to a concentration of 99.7% using molecular sieves [6].

3. Energy Integration

Using the simulation data, a pinch analysis was algebraically performed to benchmark the energy integration potential of the process. The pinch analysis allowed us to know not only the minimum requirements for heating services but also the minimum requirement for cooling services in the plant. To attain the energy targets, a heat exchange network was proposed following the criteria reported in the literature [3].

4. Environmental Assessment

For the environmental analysis the WAR GUI software, was used. This software allowed us to estimate the impacts generated in different aspects, processes, products, and raw materials of the plant [5]. To determine which scenario (base one or integrated one) had the greatest environmental impacts.

5. Results and Discussion

The simulation was performed using a calculation basis of 1,795.8 t of biomass/year, with a mixture concentration of 0.5 wet basis. Figure 1 illustrates the simulation of the plant.

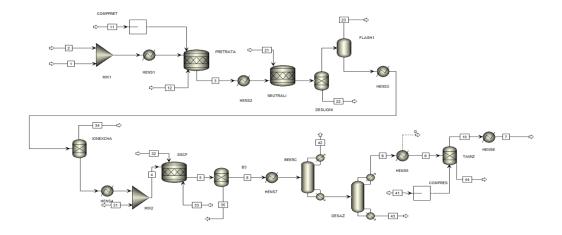


Figure 1. SSCF bioethanol plant

The feed stream was send to a pretreatment reactor where the following reactions took place [6]:

 $Hemicellulose + Water \rightarrow Xilose$ $Cellulose + Water \rightarrow Glucose$ $Lignin \rightarrow Lignin_{ac}$ After the pretreatment stage, the stream is sent downstream to a neutralization reactor where gypsum is precipitated (see Figure 1). Then it is separated of the process along with the lignin.

The table 1 shows a description of the main streams of the plant. The bioethanol left the fermentation reactor with a concentration around 6% (mass basis). Then it was sent to the purification train where, using an absorption tower, the carbon dioxide is extracted from the process stream. The separation continues with a distillation where bioethanol/water mixture reached its azeotropic point.

Stream	1	3	4	5	6	7
Mass flow (kg/h)	205	665.61	537.508	547.508	32.5	30.7
Temperature (K)	298.15	463.15	303.15	298.15	333.15	298.15
Pressure (atm)	1	13	1	1	1	1
Mass fractions						
Water	0.5	0.8357	0.853	0.8315	0.056	0.03
Lignin	0.0975	0.03568	0	0	0	0
Cellulose	0.1561	0.05588	0.0004	0.01358	0	0
Hemicellulose	0.1365	0.0026	0.000023	0.0032	0	0
Xylose	0	0.05377	0.0666	0.0098	0	0
Ethanol	0	0	0	0.06	0.944	0.997
CO_2	0	0	0	0.0568	0	0
Glucose	0	0.00578	0.055	0.0052	0	0
Furfural	0	0.0021	0.000047	0.00004	0	0
H_2SO_4	0	0.0009	0	0	0	0

Table 1. Description of the main streams

In this stage, the bioethanol reached the maximum concentration of 94.44% [8], reported that the azeotrope concentration of the ethanol-water mixture is 96.5%. However, the simulation showed that the azeotrope was formed at a lower concentration because the presence of some sub-products of the fermentation. Finally, the ethanol was purified to a concentration of 99.7%.

1.1. Energy Integration

For the pinch analysis, the streams that involved changes in their energy content by means of heat transfer in exchangers were used to the analysis. Table 2 shows the cold and hot streams selected from the process for energy integration:

Stream	$T_{s}(K)$	$T_t(K)$	$FC_p\left(\frac{kJ}{hK}\right)$	$\Delta H \left(\frac{kJ}{h}\right)$
$8(C_1)$	298.15	320.00	2,006.09	43,833.28
$9(H_1)$	351.32	333.15	56.03	-1,000.27
$10 (H_2)$	306.15	298.15	91.49	- 740.82

Table 2. Hot and Cold Streams

Figure 2 shows the Temperature Interval Diagram (TID) for the selected hot and cold streams. The energy contribution of each interval is determined by the cold and hot streams requirements (Figure 2). Table 3 and 4 shows the Table of Exchangeable Heat Loads (TEHL) contributions of heat by heating and cooling for each interval.

			T(K)	t (K)	
	Н1		351.32	341.32	
1		,	333.15	323.15	
2			330	320	C1
3			308.15	298.15	1
4		H2	306.15	296.15	
5			298.15	288.15	

Figure 2. Temperature Interval Diagram (TID)

Interval	H_1 (kJ/h)	$H_2(kJ/h)$	Total (kJ/h)
1	1,018.14	0	1,018.14
2	0	0	0
3	0	0	0
4	0	0	0
5	0	731.02	731.02

Table 3. TEHL for hot streams

Table 4. TEHL for cold streams

Interval	C_1 (kJ/h)	Total (kJ/h)
1	0	0
2	0	0
3	43,833.07	43,833.07
4	0	0
5	0	0

The data in table 3 allowed us to obtain the constraints of the model for pinch point determination and minimum heating and cooling requirements. The restrictions obtained from the model were solved using the LINGO; the following equations show the constraints.

$$1,018.14 + Q_{Heating}^{min} - r_1 = 0; (1)$$

$$r_1 - r_2 = 0;$$
 (2)

$$r_2 - 43,833.07 - r_3 = 0; (3)$$

$$r_3 - r_4 = 0;$$
 (4)

$$731.92 + r_4 - Q_{Cooling}^{min} = 0; (5)$$

$$Q_{Heating}^{min} >= 0; (6)$$

$$Q_{Cooling}^{min} >= 0; (7)$$

$$r_1 >= 0; (8)$$

$$r_2 >= 0; (9)$$

$$r_3 >= 0; (10)$$

The model solution shows that the minimum requirements for heating was 42,814.93 kJ/h and for cooling 731.92 kJ/h. The temperature at the pinch point was 308.15 K, in the hot scale.

A Heat Exchange Network (HEN) was designed to achieve the potential energy integration as proposed in his methodology [3]. The HEN allows the reduction of requirements for industrial services in the biorefinery operation. Analyzing the temperatures of hot and cold streams and taking into account the restriction $\Delta T_{min} = 10$ K, only streams C_1 and H_1 can exchange heat. Figure 3 shows the HEN proposed for this system.

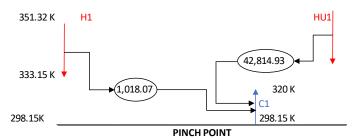


Figure 3. Heat Exchange Network Proposed

Table 5 shows the energy requirements of the process, the minimum and those reached after the energy integration.

Table 5. Industrial Process Service Requirements

Parameter	Heating	Cooling
	(kJ/h)	(kJ/h)
Energy requirements of the process	43,833	1,750
Minimal requirements	42,815	732
Maximum saving percentage	2.3 %	58.2%

It is observed that for the case without heat integration, the amount of industrial heating service is significantly higher in comparison to the cooling. The heat integration of the process did not show great savings in heating services (2.3%), as opposed to cooling, where almost 60% of savings were achieved.

1.2. Environmental Assessment

Initially, a comparison of the Potential Environmental Impact (PEI) between the base case and the integrated one was performed. The environmental assessment was carried out for each sub-process of the plant in the integrated case. Figure 6 shows the results of potential impacts for pretreatment, fermentation, and purification. For human toxicity by ingestion, the pretreatment is the stage of the process that affects this aspect the most because of the presence of substances such as sulfuric acid and/or furfural. The assessment showed that, in general, it does not exist any risk in the stages due to exposure limits for the substances involved in the process. This implies that in the operation of the plant, the workers would not be in danger during the process operation.

On the other hand, the potential for terrestrial toxicity is impacted mainly by the pretreatment and purification stage. It is evident, that one of the most important aspects to take into account when designing and operating the plant, are the possible impacts on the soil by the chemicals used in those stages of the process. Finally, the photochemical oxidation is the aspect of the operation of the plant that is affected the most by the purification stage.

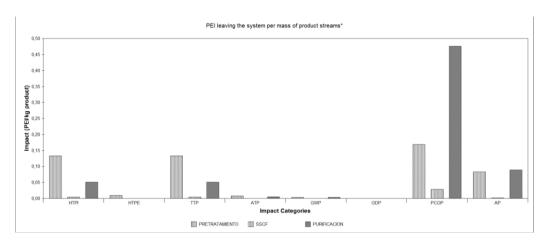


Figure 4. Environmental Assessment of PER for each stage of the process

4 Conclusions

In this study, a bioethanol production plant was simulated and analyzed from rice residues. The results showed that for the operations of the process, 0.149 kg of ethanol is produced per kg of biomass (rice residues) entering the plant, which is a significant value and shows that from solid wastes with low Market value, biofuels can be obtained.

In addition, the pinch analysis and the energy integration applied to the plant allowed us to determine the potential savings of industrial heating and cooling services, reducing production costs and optimizing available resources. The environmental analysis showed that the pretreatment stage is the one that affects the human toxicity by ingestion and the potential of terrestrial toxicity the most. This is because of the presence of substances with low lethal dose. This aspect must be taken into account during a possible design and operation of the plant. Regarding the exposure limits, the analysis indicates that the plant does not present great hazards in this aspect, which facilitates the design of contingency systems and industrial safety plans.

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