

## Exploration of Biomass for the Production of Bioethanol: “A Process Modelling and Simulation Study”

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### Abstract

Bio-ethanol is a clean and renewable fuel that is gaining a significant attention mainly due to its major environmental benefits and its production from diverse resources. The campaign for establishment of bio-refineries and encouragement of fossil fuels is gradually gaining a greater attention. In this research work, we seek to comparatively investigate the material requirement, production yield, and total equipment cost involved in the rice-husk and maize-cob transformation into the bio-ethanol fuel for a large-scale production using a process modeling and simulation study in order to promote the potential investors' interest. This analysis is carried out using a simulator (Aspen HYSYS) and a computational package (MATLAB). The evaluation entails modeling, simulating, and material and energy analysis including the process equipment sizing and cost for the plants. The comparative material analysis of the yield from the model process for the use of biomasses reveals that 9.94 kg and 7.32 kg of fuel-grade bio-ethanol is obtained using 0.03 kg and 0.02 kg of enzymes for every 1 kg of rice-husk and maize-cob charge in the plant, respectively, per hour. Analysis of the plants' energy flow shows that the maize-cob transformation into the bio-ethanol fuel requires more energy than the rice-husk-based plant, confirming that the maize-cob conversion is more energy-intensive than the rice-husk conversion. Moreover, the equipment cost analysis indicates that it costs \$4739.87 and \$1757.36 in order to process 1 kg of biomass (rice-husk and maize-cob) into fuel-grade bio-ethanol, respectively, per hour. Ultimately, the findings of this work identify the rice-husk's use to be of high yield, while maize-cob makes the production less capital-intensive.

**Keywords:** Bio-fuels, Biomass, Process Modeling, Fermentation, Hydrolysis.

### 1. Introduction

The growing environmental problems in the recent years and the need to reduce oil dependency have necessitated an increased interest in producing bio-ethanol as an alternative to the vehicle fuel. These are in addition to the octane boosting capacity and potential reduction in carbon monoxide (CO) emissions [1]. An increase in the world's energy demand and the progressive depletion of oil reserves motivate the search for alternative energy resources, especially for those derived from renewable materials such as biomass. Biomass is one of the most promising renewable resources used in order to generate different types of bio-fuels such as bio-diesel [2]. The global concern about climate change and the consequent need to diminish greenhouse gas emissions have encouraged the use of bio-ethanol as a gasoline replacement or additive. Bio-ethanol can be obtained from renewable sources

containing starch, sugar or the lignocellulosic materials such as potatoe, corn, corn cobs and stalks, grains, and wood that mainly comprise cellulose (a glucose polymer), hemicellulose, a mixture of polysaccharides mainly composed of glucose, mannose, xylose, arabinose, and lignin [2, 3].

Due to the rising demand for energy and the continuous depletion of oil reserves coupled with greenhouse emissions from non-renewable energy sources, the need for alternative clean energy fuels such as bio-ethanol is indispensable. Besides, the disposal of lignocellulose wastes causes environmental pollution in our surroundings—this improper management of solid wastes affects the human and animal health. Lignocellulose is considered as an attractive feedstock for fuel ethanol production due to its availability in large quantities, relatively low cost, and significant

reduction in the competition with food but not necessarily with feed [4, 5].

A survey of the literature indicates that several investigations have been carried out in order to provide a possible solution to get this challenge addressed. For instance, Sasser et al. [6] have evaluated the feasibility of using spruce (softwood), salix (hardwood), and corn stover (agricultural residue), and demonstrates the importance of a high ethanol yield and the necessity of utilizing the pentose fraction for ethanol production to obtain a good process economy, especially when salix or corn stover is used [7]. Christiana and Eric [8] have been able to identify that the production of bio-ethanol from cassava is only feasible in Nigeria, provided that the plant is a site next to the plant. Oyegoke et al. [9] have indicated that 143 million liters of bio-ethanol per annum can be obtained using 402 metric tonnes of sugarcane bagasse. That is 2.8 metric tonnes of sugarcane bagasse can always yield 1 million liters of bio-ethanol. Some works are related to the bio-ethanol production from molasses [10], combine sugarcane-bagasse-juice [11, 12], and sorghum bagasse [13]. In other research works, the researchers have examined the potential of converting wastes into power instead of bio-fuels. In some of these research works, Sobamowo and Ojolo [14], Oyegoke et al. [15], Abbas et al. [16], and Mataji and Shahin [17] have explored the use of municipal wastes, sugarcane bagasse, other biomass resources, and wind energy, respectively, to generate power.

In addressing the challenge of solid waste management and the promotion of a green fuel and cleaner air campaign, in this work, we

comparatively assessed the utilization of maize-cob (A) and rice-husk (B) for the bio-ethanol production using a process simulation approach. This goal was achieved via the execution of the following tasks: (1) collection of the relevant experimental data, (2) modeling and simulation of the process plant using the relevant laboratory-verified data in order to analyze the material and energy flow across the modeled process plant, (3) the equipment modeled was sized with the aid of the Aspen HYSYS process simulator, and (4) the sized equipment cost was used in order to determine the total plant equipment cost involved in the transformation of rice-husk and maize-cob in the plants A and B, respectively. This work reveals the plant yield, total equipment cost for processing 1 kg of biomass (rice-husk and maize-cob), and material and energy requirements for a biomass conversion into bio-ethanol. This information would provide the preliminary guidance for the potential investors, especially on feedstocks' choice considering their yield, energy, and cost implications in terms of the equipment cost.

## 2. Materials and Methods

In this work, we employed a PC coupled with some application software like Aspen HYSYS (for modeling and simulation of the process) and Microsoft Excel/MATLAB (for computational use). The mass basis (for the feedstock) used in this work was obtained as a fraction of what was reported by the Nigeria Bureau of Statistics for the annual total mass of maize (for cob) and rice (for husk) produced nationally, averaged for a series of recent years.

**Table 1. Components used for the bio-ethanol simulation**

| Component      | Formula                  | Use in the process                                  |
|----------------|--------------------------|---|
| Cellulose*     | $C_6H_{10}O_5$           | Feedstock   |
| Hemicellulose* | $C_5H_8O_4$              | Feedstock   |
| Sulphuric acid | $H_2SO_4$                | Acid catalyst                                       |
| Furfural       | $C_5H_4O_2$              | Hemicellulose hydrolysis by-product                 |
| Acetic acid    | $C_2H_4O_2$              | Hydrolysis and fermentation by-product              |
| Acetate*       | $C_2H_4O_2$              | Acetate groups present in hemicellulose             |
| Glucose*       | $C_6H_{12}O_6$           | From cellulose hydrolysis and saccharification      |
| Cellobiose*    | $C_{12}H_{22}O_{11}$     | From cellulose hydrolysis and saccharification      |
| Xylose*        | $C_5H_{10}O_5$           | Coming from hydrolysis and saccharification         |
| Water          | $H_2O$                   | Product moisture, washing, and the reaction product |
| Ethanol        | $C_2H_6O$                | Desired product                                     |
| Carbon dioxide | $CO_2$                   | Fermentation product                                |
| Z. mobilis*    | $CH_{1.8}O_{0.5}N_{0.2}$ | Fermentation bacteria                               |
| Glycerol       | $C_3H_8O_3$              | Fermentation by-product                             |
| Lignin*        | $C_{10}H_{13.9}O_{1.3}$  | Feedstock   |
| Xylitol*       | $C_5H_{12}O_5$           | Fermentation by-product                             |

Note: Some of the components listed above (The asterisk ones\*) are not available in the components database. These components are added as hypotheticals.

**2.1 Modelling conditions, method, and components**

In this work, we employed Aspen HYSYS in the modeling of the process in order to produce bio-ethanol from rice-husk (Plant A) and maize-cob (Plant B). In the modeling of the plants (Plants A and B), a non-random two-liquid (NRTL) thermodynamic model was selected in order to predict the thermodynamic and physical properties of the components involved in this work.

The NRTL selection has been reported by

Oyegoke & Dabai [12] to be useful due to the nature of the components. Any component not available in the Aspen database was modeled using the PubChem database information data.

The set of the components involved in this work is presented in table 1. In contrast, the details for the modeled components, commonly called the hypothetical components, are presented in tables 2 and 3 for the liquid and solid components.

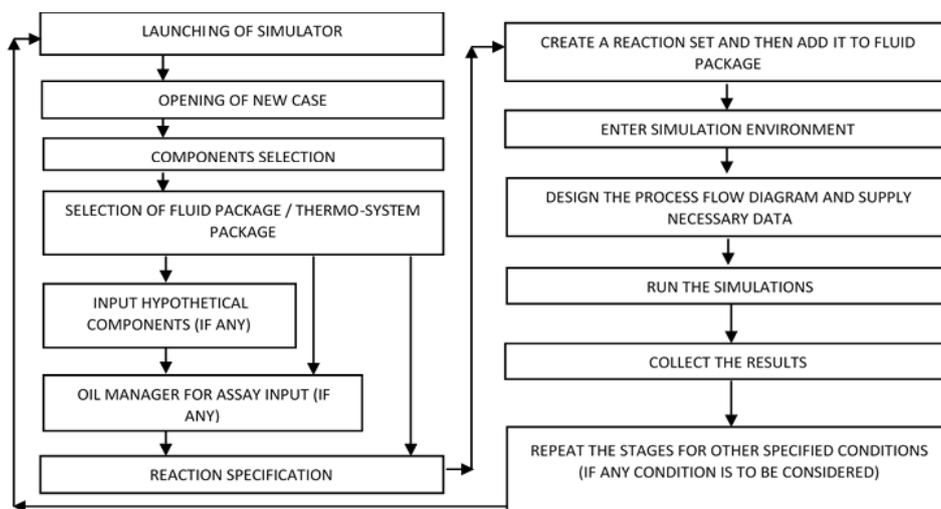
Moreover, the approach employed in the modeling and simulation of the process plant was carried out using the approach step-wisely displayed in figure 1 adopted from the literature [12]. The process simulation was done using the Aspen HYSYS simulator.

**Table 2. Liquid hypotheticals and their properties used in the HYSYS process simulator.**

| Properties           | Unit                  | Acetate | Glucose  | Cellobiose | Xylose   | Hemicellulose | Xylitol  |
|----------------------|-----------------------|---------|----------|------------|----------|---------------|----------|
| Molecular weight     | g/mol                 | 60.05   | 180.16   | 342.3      | 150.1    | 132.1         | 152.1    |
| Normal boiling point | °C                    | 118     | 343.9    | 626.9      | -382.9   | 421.2         | 421.2    |
| Ideal liq. density   | kg/m <sup>3</sup>     | 1052    | 1269     | 1514       | 1288     | 894.7         | 894.7    |
| Critical temperature | °C                    | 319.6   | 737.9    | 961.9      | 642.4    | 759.8         | 759.8    |
| Critical pressure    | kPa                   | 5770    | 6200     | 3921       | 6588     | 6320          | 6320     |
| Critical vol.        | m <sup>3</sup> /kgmol | 0.1710  | 0.4165   | 0.778      | 0.388    | 0.3990        | 0.3990   |
| Accentricity         |                       | 0.4470  | 2.567    | 0.8442     | 0.706    | 0.5651        | 0.5651   |
| Ht. of formation     | kJ/kgmol              | -435079 | -1256903 | -625070    | -1040020 | -241287.3     | kJ/kgmol |
| Ht. of combustion    | kJ/kgmol              | -786425 | 2817760  | -          | 0.002352 | -             | kJ/kgmol |

**Table 3. Solid hypotheticals and their properties used in HYSIS process simulator.**

| Properties                  | Unit              | Cellulose | Lignin   | Z-mobilis |
|-----------------------------|-------------------|-----------|----------|-----------|
| Molecular weight            | g/mol             | 162.1406  | 122.49   | 24.63     |
| Density                     | kg/m <sup>3</sup> | 1500      | 1500     | 1500      |
| Heat of formation (25 °C )  | kJ/kgmol          | -963000   | -1592659 | -130500   |
| Heat of combustion (25 °C ) | kJ/kgmol          | -2828000  | 3265480  | 520125    |



**Figure 1. Flow chart for simulating a process in Aspen HYSYS [12].**

## 2.2 Feedstocks and reaction set involved in this work

The chemical composition of the feeds charged into the two plants is presented in tables 4 and 5,

both obtained by averaging the feedstock's two cited compositions.

**Table 4. Cellulose, hemicellulose, and lignin content in rice-husk.**

| Cellulose | Hemicellulose | Lignin | Reference                            |
|-----------|---------------|--------|--------------------------------------|
| 15-36     | 12-35         | 8-16   | Saha & Cotta [18]; Saha & Cotta [19] |
| 25-35     | 18-21         | 26-31  | Rabemanolontsoa & Saka [20]          |
| 27.8      | 21.5          | 20.3   | Average                              |

**Table 5. Cellulose, hemicellulose, and lignin content in maize-cob.**

| Cellulose | Hemicellulose | Lignin | Reference                   |
|-----------|---------------|--------|-----------------------------|
| 45        | 35            | 15     | Sun & Cheng [21]            |
| 42-45     | 35-39         | 14-15  | Rabemanolontsoa & Saka [20] |
| 44        | 36.7          | 13.2   | Average                     |

In this work, the bio-ethanol production steps employed were as follow: pre-treatment, hydrolysis, pH adjustment/neutralization, and fermentation. The reaction sets characterizing these steps are present in table 6. These reaction sets present the series of reactions modeled in a reactor. First was the pre-treatment hydrolyzer reaction set (1), which was modeled in the pre-treatment unit. Moreover, the hydrolysis reaction set (2) was modeled within the hydrolyzer, converting the polysaccharide into the monosaccharides like xylose and glucose in the

presence of sulfuric acid. The pH adjustment reaction set (3) was modeled in order to initiate the neutralization reaction used to neutralize the acid content present in the simple sugar produced in the hydrolyzer. Another reaction set is fermentation reactions (4), which entail a set of reactions that experimentally occur within a fermenter during the sugar conversion into bio-ethanol. All the reaction sets occur in separate reactors except for the process of simultaneous saccharification and fermentation (SSF), which combines the reaction sets (2) and (4).

**Table 6. The reaction sets employed in this work.**

| Reaction sets  | Reaction expressions/equations  |
|--|---|
| (1) Pre-treatment hydrolyzer reaction(s)                                   | $\text{Cellulose} + \text{H}_2\text{O} \rightarrow \text{Glucose}$                                |
|  | $\text{Cellulose} + 0.5 \text{H}_2\text{O} \rightarrow 0.5 \text{Cellobiose}$                     |
|  | $\text{Hemicellulose} + \text{H}_2\text{O} \rightarrow \text{Xylose}$                             |
|  | $\text{Hemicellulose} \rightarrow \text{Furfural} + 2 \text{H}_2\text{O}$                         |
|  | $\text{Acetate} \rightarrow \text{Acetic acid}$   |
| (2) Hydrolysis reaction(s)   | $\text{Sucrose} + \text{H}_2\text{O} \rightarrow 2 \text{Glucose}$                                |
|  | $\text{Cellulose} + \text{H}_2\text{O} \rightarrow 90 \text{Glucose}$                             |
|  | $\text{Cellulose} + 0.5 \text{H}_2\text{O} \rightarrow 0.5 \text{Cellobiose}$                     |
|  | $\text{Cellobiose} + \text{H}_2\text{O} \rightarrow 90 \text{Glucose}$                            |
|  | $\text{Cellulose} + \text{H}_2\text{O} \rightarrow 90 \text{Glucose}$                             |
|  | $\text{Cellulose} + 0.5 \text{H}_2\text{O} \rightarrow \text{Cellobiose}$                         |
|  | $\text{Hemicellulose} + \text{H}_2\text{O} \rightarrow 64 \text{Xylose}$                          |
| $\text{Hemicellulose} \rightarrow \text{Furfural} + 47 \text{H}_2\text{O}$ |   |
| (3) pH adjustment reaction   | $2 \text{NaOH} + \text{H}_2\text{SO}_4 \rightarrow \text{Na}_2\text{SO}_4 + 2 \text{H}_2\text{O}$ |
| (4) Fermentation reaction(s)   | $\text{Glucose} \rightarrow 3 \text{Ethanol} + \text{CO}_2$                                       |
|  | $3 \text{Xylose} \rightarrow 2 \text{Ethanol} + \text{CO}_2$                                      |
|  | $\text{Glucose} + \text{H}_2\text{O} \rightarrow 0.2 \text{Glycerol} + \text{O}_2$                |
|  | $\text{Xylose} + 5 \text{H}_2\text{O} \rightarrow \text{Glycerol} + 4.6 \text{O}_2$               |

During the pre-treatment hydrolyzer reaction(s), there is some partial hydrolysis of the feed in which a significant fraction of hemicellulose is hydrolyzed. In contrast, the hydrolysis reaction(s) involve the breaking down of sucrose, hemicellulose, and cellulose into glucose and xylose in the presence of water at a temperature of 394 K. In a neutralization reaction, all the acidic content of the hydrolyzed products is neutralized

to the barest minimum. Finally, the fermentation reaction(s) convert glucose and xylose to ethanol and carbon dioxide in the presence of enzymes at a temperature of 394 K.

## 2.3 Process flow development

In a literature review [22–27], two different routes were identified for bio-ethanol production from lignocellulosic biomass (for the use of rice-husk

and maize-cob). The first route was a simultaneous saccharification and fermentation, which was chosen for bio-ethanol production from rice-husk due to the reported high bio-ethanol yield, low quantity of enzyme requirement, reduced contamination, low inhibition, and low cost. The second route was a separate hydrolysis and fermentation, which was chosen to produce bio-ethanol from maize-cob because the hydrolysis and fermentation processes occurred under the optimum conditions.

## 2.4 Process Description

**Plant A:** The rice-husk with the composition shown in table 4 at 180 kg/h, 25°C, and 101.3 kPa, and water at 90 kg/h, 25 °C, and 101.3 kPa were mixed in a mixer and heated to 121 °C at 1605 kg/h and 101.3 kPa, and were fed together into the acid pre-treatment reactor, where dilute sulfuric acid at 90 kg/h, 25 °C, and 101.3 kPa was fed (Reaction set 1 in table 6).

The products from the acid pre-treatment reactor were first heated to 121 °C, and then fed into the acid hydrolysis (Reaction set 2 in table 6) and fermentation (Reaction set 4 in table 6) reactor together with dilute sulfuric acid at 90 kg/h, 25°C, and 101.3 kPa, and enzyme (91.68% water) at 5.94 kg/h, 121°C, and 101.3 kPa.

The products from the dilute acid hydrolysis and fermentation (SSF) reactor were fed into a filter, where the products were filtered into a solid fraction and a liquid fraction. The liquid fraction, i.e. the filtrate, was sent to the pH adjustment reactor (Reaction set 3 in table 6) using NaOH in order to neutralize the acidity. The pH adjustment reactor effluent was cooled to 30 °C and sent to the purification section. Figure 2 shows the block flow diagram for producing bio-ethanol from rice-husk using the selected routes.

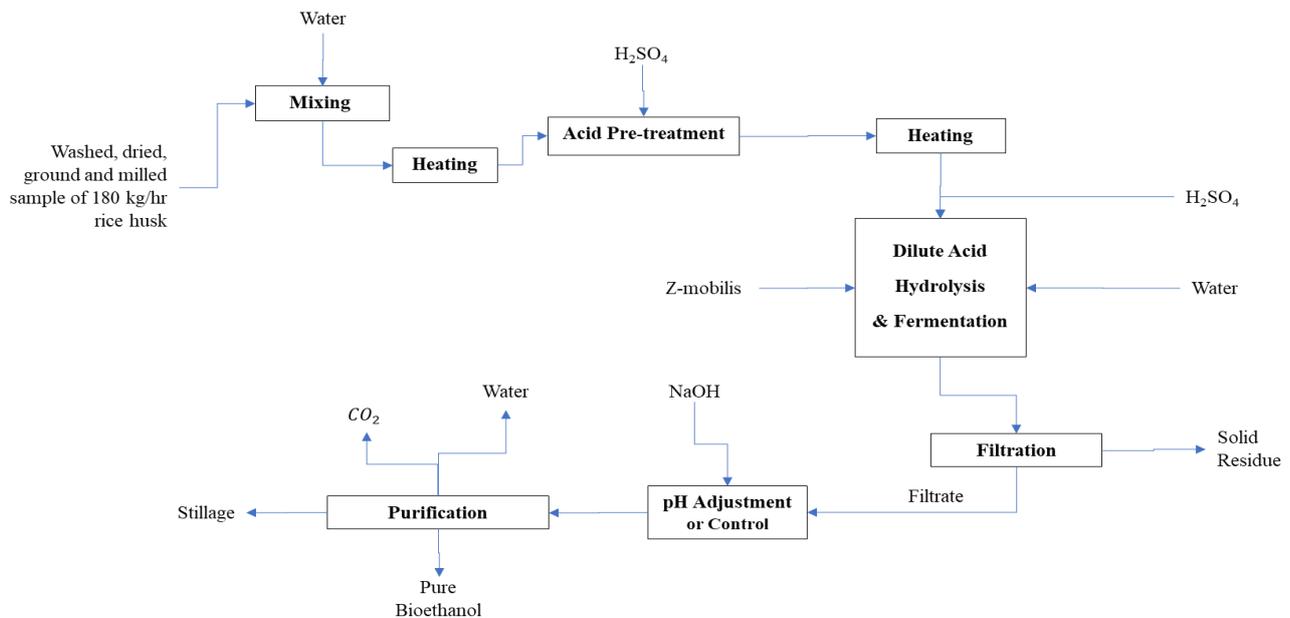


Figure 2. Production of bio-ethanol in plant A.

**Plant B:** The feedstock, corn cob whose composition is presented in table 5 at 567.3 kg/h, 25 °C, 101.3 kPa, and water at 1021 kg/h, 25 °C, and 101.3 kPa, was mixed in a mixer and heated to 121 °C at 1080 kg/h, 101.3 kPa; these were fed together into the pre-treatment reactor (Reaction set 1 in table 6), where sulfuric acid at 17.02 kg/h, 25 °C, and 101.3kPa was fed. The products from the pre-treatment reactor were cooled to 98°C and fed together with water at 1021 kg/h, 101.3 kPa, and 25 °C and dilute sulphuric acid at 51.34 kg/h, 25°C, and 101.3 kPa into the dilute acid

hydrolysis reactor, where the saccharification reaction (Reaction set 2 in table 6) took place.

The dilute acid hydrolysis reactor products were fed together with an enzyme (91.68 % water) at 11.35 kg/h, 121°C, and 101.3 kPa into the fermentation reactor, where the fermentation took place (Reaction set 4 in table 6). The fermentation reactor products were fed into a filter, where it filtered the products into a solid fraction and a liquid fraction. The liquid fraction, i.e. the filtrate, was sent to the pH adjustment reactor (Reaction set 3 in table 6) using NaOH in order to neutralize its acidity. The pH adjustment reactor effluent was

cooled to 30 °C and sent to the purification section. Figure 3 shows the block flow diagram to

produce bio-ethanol from maize-cob using the selected routes.

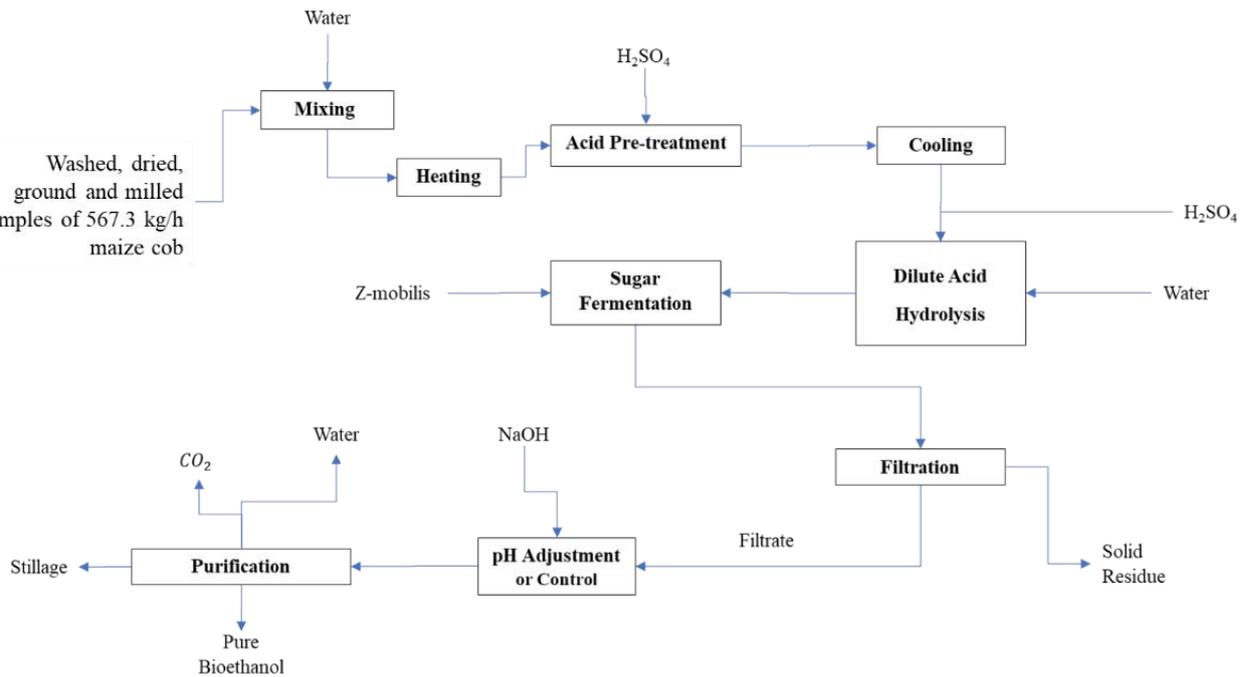


Figure 3. Production of bio-ethanol in plant B.

In the purification section, a separator was used in order to separate CO<sub>2</sub> from the beer. CO<sub>2</sub> was sent to a 10-stage absorption column with the feed entering at stage 4 to wash CO<sub>2</sub> before releasing into the atmosphere, and the beer was channeled to a different absorption column with steam in order to remove the stillage (waste). Two products were obtained from the beer refinement; the light one was sent to a refluxed absorber, while the concentrated one was sent to the distillation column. The condenser pressure was set to 101.3 kPa. Two specifications were made: an overhead vapor rate 69 kg/h and an ethanol component mass fraction. The liquid was fed into a 29-stage distillation column with the feed entering at stage 12. The condenser and reboiler pressures were kPa 172.3 and 202.6 kPa, respectively. At the full reflux condenser, two specifications were added. The specification included setting the reflux ratio to be 1.241 and its flow rate to be 38940 kg/h (in the process plant modeling) to give a 95% purity (for bio-ethanol) during the distillation process. It is noteworthy that the same purification procedure used for the bioethanol production in plant A (rice-husk) was adopted here for plant B (maize-cob).

### 2.5 Material and energy balance analysis

The material and energy flow stream across the process equipment and the entire plant modeled

were evaluated in order to ensure that the energy and mass were conserved [28, 29]. Overall, the plant material and energy analysis helped to identify the material and energy required to keep the plant running, while the overall process equipment balance aided in designing the process equipment. The general material balance equation is given as:

$$\text{Material in} = \text{Material out} + \text{Generation} - \text{Consumption} - \text{Accumulation} \quad (1)$$

In this work, the material and energy balance for the two plants was carried out with the aid of the process simulator (Aspen HYSYS), and overall, the plant-wide energy balance flow was collected for both plants.

### 2.6 Process equipment sizing and costing

The equipment sizing was done using Aspen HYSYS, and subsequently, the cost of the plant equipment was estimated. Each equipment was costed via the use of the cost relations presented in Sinnott [28] and Seider & Seader [29], which could be written as follow:

$$C_0 = a + bS^n \quad (2)$$

$$C_0 = aS^b \quad (3)$$

where S is the equipment design parameter, n is the exponent for the type of equipment, a and b are the cost constants, and C<sub>0</sub> is the base cost (at a

specified year). The estimated base cost,  $C_0$ , was updated to the current year via the relation presented in Equation 4 using the cost index table/chart.

$$\frac{C_0}{I_0} = \frac{C_N}{I_N} \quad (4)$$

where  $I_0$  and  $I_N$  are the base and current chemical engineering plant cost index and  $C_N$  is the current cost for the year of study. Summing the cost of all equipment, the total plant equipment cost was evaluated. The details of the computations are shown in Appendix B.

### 3. Research Findings and Discussions

#### 3.1 Process Flow Sheet Model

The process flow diagrams modeled for the process information presented in the block flow diagrams in figures 2 and 3 are shown in figures 4 and 5, respectively.

#### 3.2 Material Balance Analysis

The material balance analysis of the proposed plants is shown in table 7. It can be seen that 1,789.45 kg/h of 99% pure bio-ethanol can be produced from 180 kg/h pre-treated, washed, and crushed feed of rice-husk. Similarly, 4,154.94 kg/h of 99 % pure bio-ethanol could be produced

from 567.3 kg/h pre-treated, washed, and crushed feed of maize-cob using 5.94 kg enzyme/h and 11.35 kg enzyme/h, respectively.

Furthermore, in this work, indicates that a kilogram of rice-husk and maize-cob would yield 9.94 kg (1789.45 kg/180 kg) and 7.32 kg (4154.94 kg/567.30 kg) of fuel-grade bio-ethanol using 5.94 kg and 11.35 kg of enzymes, respectively, in every hour. These findings indicate that the amount of yield obtained for the use of rice-husk and maize-cob is higher than the values reported for the use of rice-hull as 0.27 kg (347.25 L/t) by Quintero and Cardona [30], cassava as 0.34 kg by Christiana and Eric [8], rice-husk as 0.20 kg by Quintero et al. [31], sugarcane bagasse as 0.28 kg by Oyegoke et al. [9], molasses as 0.12 kg by Abemi et al. [10], combined use of sugarcane bagasse-juice as 0.29 kg by Oyegoke & Dabai [11], and sorghum as 0.27 kg by Ajayi et al. [13]. The yield obtained for the use of rice-husk in these studies show a higher yield compared to the ones obtained by Quintero and Cardona [30] and Quintero et al. [31], that have used the same rice hull and husk but a different technique of using the SHF approach, unlike what was adopted for this work. However, this work implies that both maize-cob and rice-husk display a high yield based on the conditions employed.

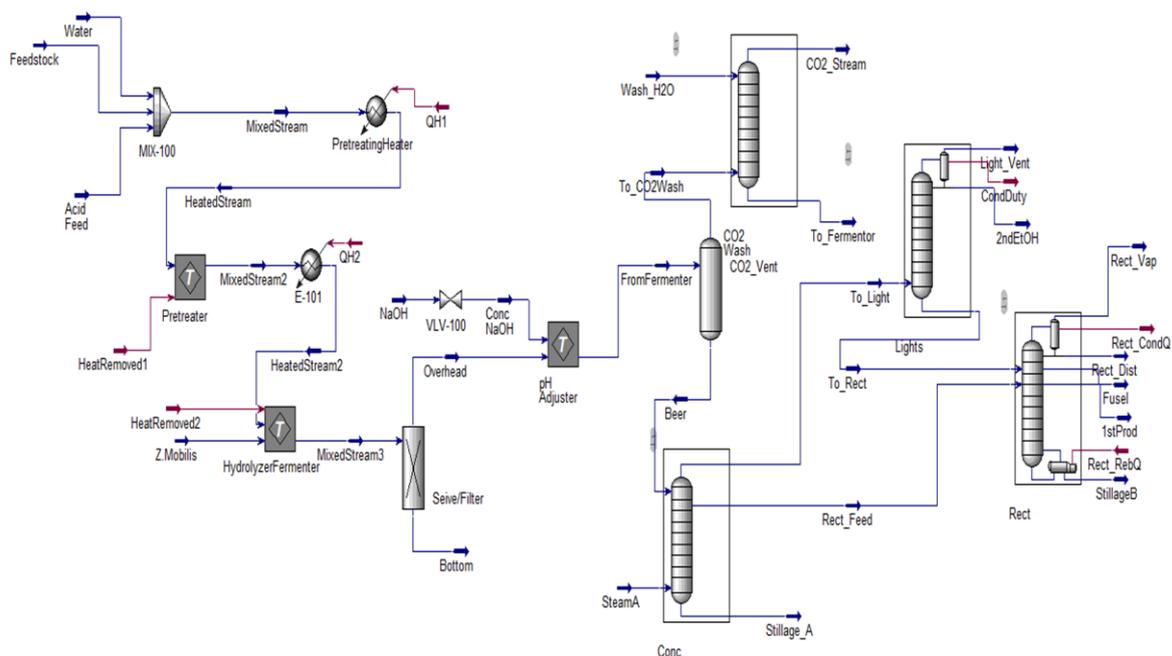


Figure 4. Process flow diagram for bio-ethanol production from rice-husk (plant A).

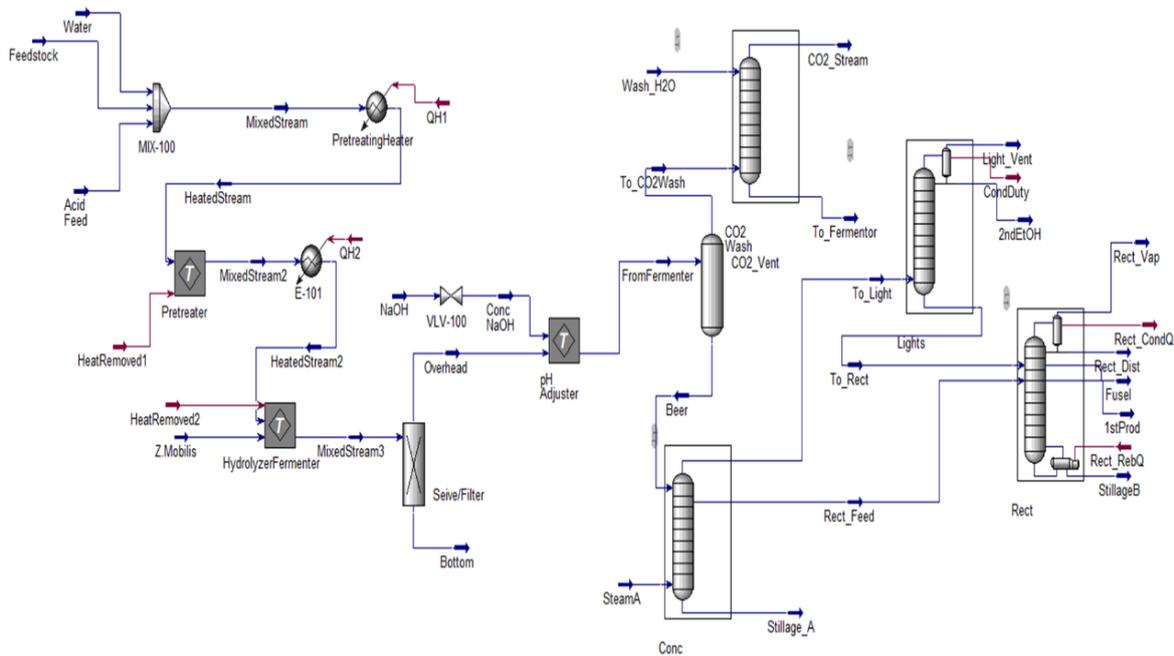


Figure 5. Process flow diagram for bio-ethanol production from maize-cob (plant B).

Table 7. Overall material balance across plants.

| Plant A           |             |                            |             | Plant B           |             |                            |             |
|-------------------|-------------|----------------------------|-------------|-------------------|-------------|----------------------------|-------------|
| Inlet material    | Flow (kg/h) | Outlet material            | Flow (kg/h) | Inlet material    | Flow (kg/h) | Outlet material            | Flow (kg/h) |
| (1) Sulfuric acid |             | (1) Other streams          |             | (1) Sulfuric acid |             | (1) Other streams          |             |
| Acid feed         | 23.50       | Bottom 3                   | 285.00      | Acid feed         | 17.02       | Solids                     | 120.92      |
| Acid feed 2       | 66.50       | Stillage-A                 | 698.6       | Acid feed 2       | 51.34       | Bottom                     | 571.37      |
| (2) Biomass       |             | Stillage B                 |             | (2) Biomass       |             | Stillage- A                |             |
| Rice husk         | 180.00      | Fusel                      | 3.00        | Maize-cob         | 567.30      | Stillage B                 | 966.5075    |
| (3) Water         |             | Rect_Dist                  |             | (3) Water         |             | Rect_Dist                  |             |
| Water             | 810.00      | (1) Light gases            |             | Water             | 1021.00     | Fusel                      | 3.00        |
| Wash_H2O          | 13.10       | CO2_stream                 | 23.89       | Wash_H2O          | 28.17       | (2) Light gases            |             |
| Steam A           | 2270.23     | Light_Vent                 | 43.91       | Steam A           | 5515.94     | CO2_stream                 | 39.89       |
| (4) Neutralizer   |             | Rect_Vap                   |             | (4) Neutralizer   |             | Rect_Vap                   |             |
| NaOH              | 90.000      | (1) Bio-ethanol            |             | NaOH              | 36.67       | Light_Vent                 | 68.89       |
| (5) Enzyme        |             | 2ndEtOH(< 99%)             |             | (5) Enzyme        |             | (3) Bio-ethanol            |             |
| Z. Mobilis        | 5.94        | 1 <sup>st</sup> Prod (99%) | 1789.45     | Z. mobilis        | 11.35       | 1 <sup>st</sup> Prod (99%) | 4154.94     |
| Total             | 3459.30     | Total                      | 3459.30     | Total             | 7248.79     | Total                      | 7248.79     |

### 3.3 Energy Balance Analysis

Table 8 shows the energy balance analysis for fuel-grade bio-ethanol production from rice-husk and maize-cob in plants A and B. It can be seen that the hydrolysis reaction(s) of cellulose and hemicellulose are highly exothermic i.e. excess heat is giving off. The heat(s) released (i.e. “Heatremoved1” and “Heatremoved2”) are 7.29 million kJ/h and 99.8 million kJ/h for the use of rice-husk and 87.2 million kJ/h and 1.053 million kJ/h for the use of maize-cob. The monosaccharide fermentation reaction is also an exothermic reaction, which releases heat (i.e. “Heatremoved3”) of 11.2 kJ/h million and 13.6 million kJ/h for the use of rice-husk and maize-cob, respectively. However, the hydrolysis of

sucrose is an endothermic reaction process that requires 498 thousand kJ/h and 551 thousand kJ/h of energy (i.e. “Heatadded”) for the use of rice-husk and maize-cob, respectively.

The overall plant energy balance deduces that the process ‘energy flow in,’ which represents the total quantity of heat that flows into the plants, is worth 1.11 billion kJ/h and 1.23 billion kJ/h for the use of rice-husk (plant A) and maize-cob (plant B), respectively. Moreover, the study indicated that the overall energy flow of 1.11 billion kJ/h and 1.23 billion kJ/h computed for rice-husk and maize-cob, respectively, is higher than the values reported in the literature. Oyegoke *et al.* [9], Abemi *et al.* [10], Oyegoke & Dabai (2018), and Ajayi *et al.* [13] obtained values of

1.02 billion, 909.5 million, 1.08 billion, and 624 million kJ/h using sugarcane bagasse, molasses, combined use of sugarcane-bagasse-juice, and sorghum bagasse, respectively.

An error of 0.03% was found for plant A, and 0.02% for plant B was obtained for the energy analysis, which could be traced to the hypothetical components (modeled) during the simulation in line with previous reports [10, 13], which associate it to the same factor. However, the error

level obtained was higher than that reported by Oyegoke & Dabai [11] and Oyegoke *et al.* [9] as 0.01 % for the combined-use of sugarcane-bagasse-juice and sugarcane bagasse, respectively. In contrast, the error obtained for this study was found to be less than that obtained for the use of sorghum bagasse (0.06 %), as reported by Ajayi *et al.* [13] in the analysis of the energy flow in the plant network.

**Table 8. A plant-wide energy balance analysis across the plants.**

| Plant A                   |            |                            |            | Plant B                   |            |                            |            |
|---------------------------|------------|----------------------------|------------|---------------------------|------------|----------------------------|------------|
| Inlet stream              | Flow (J/h) | Outlet stream              | Flow (J/h) | Inlet stream              | Flow (J/h) | Outlet stream              | Flow (J/h) |
| (1) Energy of material in |            | (1) Energy of material out |            | (1) Energy of material in |            | (1) Energy of material out |            |
| Acid feed                 | -7.33E+03  | Bottom 3                   | -9.50E+05  | NaOH                      | -7.65E+04  | Solids                     | -1.19E+06  |
| Feedstock                 | -1.22E+03  | CO2_Stream                 | -6.31E+05  | Acid feed                 | -1.39E+05  | Bottom                     | -5.69E+04  |
| Water                     | -1.28E+05  | Stillage_A                 | -4.05E+07  | Feedstock                 | -2.99E+06  | CO2_Stream                 | -2.31E+07  |
| NaOH                      | -1.88E+05  | 2ndEtOH                    | -1.85E+06  | Water                     | -1.61E+07  | Stillage_A                 | -3.84E+08  |
| Wash_H2O                  | -3.70E+05  | Light_Vent                 | -5.69E+05  | Wash_H2O                  | -3.70E+07  | 2ndEtOH                    | -1.85E+06  |
| SteamA                    | -1.45E+07  | Rect_Vap                   | -2.31E+04  | SteamA                    | -2.45E+08  | Light_Vent                 | -5.69E+05  |
| Z. Mobilis                | -3.13E+04  | StillageB                  | -6.77E+07  | Z. mobilis                | -5.99E+04  | StillageB                  | -5.19E+07  |
| (2) Heating duties        |            | 1stProd                    | -2.32E+08  | Acid feed 2               | -2.46E+08  | 1stProd                    | -3.99E+07  |
| QH1                       | 5.26E+08   | Fusel                      | -2.02E+08  | (2) Heating duties        |            | Fuel                       | -2.20E+04  |
| QH2                       | 3.90E+08   | (2) Cooling duties         |            | Heatadded                 | 5.51E+05   | Rect_Vap                   | -2.33E+04  |
| Rect_RebQ                 | 3.27E+08   | CondDuty                   | 4.57E+08   | QH1                       | 6.73E+08   | Rect_Dist                  | -1.26E+04  |
| Heatadded                 | 4.98E+05   | Rect_CondQ                 | 4.40E+08   | Rect_RebQ                 | 4.27E+08   | (2) Cooling duties         |            |
| (3) Cooling duties        |            | Rect_Dist                  | 8.99E+08   | QA                        | 7.81E+08   | QC1                        | 2.66E+08   |
| Heatremoved1              | -7.29E+06  |                            |            | (3)Cooling duties         |            | QC2                        | 8.15E+08   |
| Heatremoved2              | -9.98E+07  |                            |            | QM2                       | -9.27E+05  | CondDuty                   | 6.55E+08   |
| Heatremoved3              | -1.12E+07  |                            |            | Heatremoved1              | -8.72E+07  | Rect_CondQ                 | 4.04E+07   |
|                           |            |                            |            | Heatremoved3              | -1.36E+07  |                            |            |
|                           |            |                            |            | Heatremoved2              | -1.05E+06  |                            |            |
| Total                     | 1.11E+09   | Total                      | 1.11E+09   | Total                     | 1.23E+09   |                            | 1.23E+09   |
| Error (%)                 |            |                            | 0.03       | Error (%)                 |            |                            | 0.02       |

### 3.4 Estimation of process plant equipment cost

The result of the process plant equipment cost estimated via cost relations and index for updating the price of equipment to the current year is summarized in table 9, displaying the plant purchased equipment cost before and after the update process.

The estimation indicated that the bio-ethanol produced via rice-husk and maize-cob as their feedstock would require a total cost of \$853 thousand and \$997 thousand to transform the biomass into the fuel-grade bio-ethanol (99% purity). The findings imply that maize-cob (plant B) could require more funds to buy equipment to set up than rice-husk (plant A).

However, evaluating the result based on processing a kilogram of the biomass (rice-husk and maize-cob) into bio-ethanol indicated that it would cost \$4,739.87 (\$853176.20/180.00 kg) and \$1,757.36 (\$996950.10/567.30 kg) to purchase the process equipment for the establishment of a plant

for processing of 1 kg of biomass into the bio-ethanol fuel. In contrast, the total cost estimated for producing a kilogram of bio-ethanol was far greater than stated as 0.01626, 0.0612, and 179.1829 \$/kg in the report of molasses, sugarcane (bagasse-juice), and sorghum bagasse, respectively.

### 4. Conclusions

In the present work, we showed that agricultural waste such as rice-husk and maize-cob could be used as a feedstock or substrate for the bio-ethanol production using two different routes. Moreover, the findings from the material balance analysis indicate that the use of 180 kg/h of rice-husk produces 1,789 kg/h of fuel-grade bio-ethanol using 5.94 kg/h of enzyme. In contrast, 567.3 kg/h of maize-cob produces 4,154.94 kg/h of fuel-grade bio-ethanol using 11.35 kg/h of enzyme. Furthermore, the findings of this work reveal that a kilogram of rice-husk and maize-cob yields 9.94

kg and 7.32 kg of fuel-grade bio-ethanol using 0.03 kg and 0.02 kg of enzymes, respectively, in every hour. The overall plant energy balance analysis shows that plant B (maize-cob) requires more energy than plant A (rice-husk); that is, the maize-cob transformation into bio-ethanol require more energy during the plant operation than that of the rice-husk plant. The equipment cost analysis shows that it costs \$4,739.87 and \$1,757.36 to process a kilogram of biomass (rice-husk and maize-cob) into fuel-grade bio-ethanol, respectively, in an hour.

Although the use of rice-husk shows a higher yield (i.e. 9.94 kg bio-ethanol/kg biomass) and a lower energy input (1.11 billion kJ/h), it requires more funds (\$4,739.87/kg biomass) to purchase the start-up equipment when compared to the use of maize-cob that required \$1,757.36/kg biomass to get started. Also this study's findings identified the rice husk's use to be of high yield, while maize-cob makes the production less capital-intensive.

**Table 9. Purchased equipment cost summary for different plants.**

| Plant Description                | A          |            | B          |            |
|----------------------------------|------------|------------|------------|------------|
|                                  | $C_0$ (\$) | $C_n$ (\$) | $C_0$ (\$) | $C_n$ (\$) |
| Mixer                            | 450790.50  | 484977.40  | 348594.50  | 375031.10  |
| Heater                           | 11223.20   | 14304.50   | 12525.00   | 15962.50   |
| Reactor                          | 160602.90  | 205469.30  | 385882.00  | 493682.50  |
| Column                           | 1382.80    | 1769.20    | 1382.80    | 1769.20    |
| Separator                        | 75329.00   | 96373.10   | 75329.00   | 96373.10   |
| Molecular Sieve                  | 1138.61    | 1225.00    | 257.55     | 277.10     |
| Condenser                        | 5911.66    | 6327.70    | 5911.66    | 6327.70    |
| Reboiler                         | 6996.28    | 7526.90    | 6996.28    | 7526.90    |
| Cooler                           | 27620.00   | 35203.10   | -          | -          |
| Total cost                       | 734694.95  | 853176.20  | 836878.79  | 996950.10  |
| Total cost per kg of bio-ethanol | -          | 4739.87    | -          | 1757.36    |

**5. Recommendations**

Further studies can look into the thermodynamic analysis (energy, exergy, and pinch analysis) of the process in order to understand the plants' energy efficiency, identify the potential units mainly contributing to the plant's loss in energy, and better ways to resolve it. Also future research works can be carried out in order to investigate the use of algae for bio-ethanol production, assessing its energy efficiency, economic viability, production yield, and other issues related to the plant scale-up.

**6. Nomenclature**

- $C_0$  Base cost (at a specified year)
- $C_N$  Current cost for the year of study
- $D_{M101}$  Diameter of the mixer
- $H_{M101}$  Height of the mixer
- $I_0$  Base chemical engineering plant cost index
- $I_N$  Current chemical engineering plant cost index
- $M'$  Total mass flow rate of the mixture
- $V_{D101}$  Required size of the mixer

- a & b Cost constants
- A Area required
- A Maize-cob for plant A
- AC Absorption column
- B Rice-husk for plant B
- CD Condenser
- CL Cooler
- D Vessel diameter
- DC Distillation column
- H Heat load
- HT Heat exchanger
- L Length
- M1 Molecular sieve/Filters like M2, M3
- MX Mixer
- n Exponent for the type of equipment
- N Number of tubes
- NRTL Non-random two-liquid thermodynamic model
- P Vessel pressure
- Q Duty
- R1 Reactors like R2, R3

|     |                                 |              |   |
|-----|---------------------------------|--------------|---|
| RAC | Rectification/Absorption column | Tv           | Tray volume                                       |
| RB  | Reboiler                        | v            | Liquid volume                                     |
| S   | Rhe equipment design parameter  | V            | Volumetric flow rate of the mixture/Vessel volume |
| S1  | Separator                       | $\Delta T_m$ | Overall heat transfer coefficient                 |
| Tm  | Log mean temperature            |              |   |
| Ts  | Tray spacing                    |              |   |

## 7. Appendix

### Equipment specification results for plants A and B

Mixer sizing and specification for plants A and B

**Table A1. Summary of mixer 1 specifications**

| S/N | Parameters                               | A                        | B                       |
|-----|--|--------------------------|-------------------------|
|     |  | Values                   | Values                  |
| 1   | Total mass flow rate of the mixture $M'$ | 1080 kg/h                | 1605 kg/h               |
| 2   | Volumetric flow rate of the mixture $V$  | 0.9941 m <sup>3</sup> /h | 1.528 m <sup>3</sup> /h |
| 3   | Required size of the mixer $V_{D101}$    | 3.7 m <sup>3</sup>       | 5.7 m <sup>3</sup>      |
| 4   | Diameter of the mixer $D_{M101}$         | 1.6 m                    | 1.8 m                   |
| 5   | Height of the mixer $H_{M101}$           | 1.9 m                    | 2.2 m                   |

**Table A2. Summary of heater 1 specifications**

| S/N | Parameters                                     | A                            | B                            |
|-----|--|------------------------------|------------------------------|
|     |  | Values                       | Values                       |
| 1   | Heat load H                                    | 598 kW                       | 790 kW                       |
| 2   | log mean temperature Tm                        | 80 °C                        | 80 °C                        |
| 3   | Overall heat transfer coefficient $\Delta T_m$ | 750 W/m <sup>2</sup> °C      | 750 W/m <sup>2</sup> °C      |
| 4   | Area required A                                | 10.5 m <sup>2</sup>          | 13.9                         |
| 5   | Length L                                       | 4.83 m                       |                              |
| 6   | Number of tubes N                              | 28                           |                              |
| 7   | Duty Q   | 2.153 × 10 <sup>5</sup> kJ/h | 2.843 × 10 <sup>5</sup> kJ/h |

**Table A3. Summary of heater 1 specifications**

| S/N | Parameters                                     | A                            | B      |
|-----|--|------------------------------|--------|
|     |  | Values                       | Values |
| 1   | Heat load H                                    | 35.1944 kW                   | -      |
| 2   | log mean temperature Tm                        | 38 °C                        | -      |
| 3   | Overall heat transfer coefficient $\Delta T_m$ | 950 W/m <sup>2</sup> °C      | -      |
| 4   | Area required A                                | 1.0 m <sup>2</sup>           | -      |
| 5   | Length L                                       | 1.12 m                       | -      |
| 6   | Number of tubes N                              | 24                           | -      |
| 7   | Duty Q   | 1.267 × 10 <sup>5</sup> kJ/h | -      |

Pre-treater sizing and specifications for plants A and B

**Table A4. Summary of pre-treater specifications**

| S/N | Parameters        | A                    | B                    |
|-----|-------------------|----------------------|----------------------|
|     |                   | Values               | Values               |
| 2   | Vessel volume V   | 2.982 m <sup>3</sup> | 1.146 m <sup>3</sup> |
| 3   | Vessel diameter D | 1.363 m              | 0.9908 m             |
| 4   | Liquid volume v   | 1.494 m <sup>3</sup> | 0.764 m <sup>3</sup> |
| 5   | Vessel pressure P | 101.3 kPa            | 101.3 kPa            |
| 6   | Height H          | 2.044 m              | 1.486 m              |

Hydrolysis/Fermentation reactor sizing and specifications for A and hydrolysis reactor for B

**Table A5. Summary of pre-treater specifications**

| S/N | Parameters        | A                    | B                   |
|-----|-------------------|----------------------|---------------------|
|     |                   | Values               | Values              |
| 2   | Vessel volume V   | 72.72 m <sup>3</sup> | 3.5 m <sup>3</sup>  |
| 3   | Vessel diameter D | 3.952 m              | 1,428 m             |
| 4   | Liquid volume v   | 36.36 m <sup>3</sup> | 1.750m <sup>3</sup> |
| 5   | Vessel pressure P | 101.3 kPa            | 101.3 kPa           |
| 6   | Height H          | 5.928 m              | 2.156 m             |

pH adjuster sizing and specifications for plants A and B

**Table A6. Summary of pH adjuster specifications**

| S/N | Parameters        | A                     | B                     |
|-----|-------------------|-----------------------|-----------------------|
|     |                   | Values                | Values                |
| 2   | Vessel volume V   | 0.773 m <sup>3</sup>  | 1.030 m <sup>3</sup>  |
| 3   | Vessel diameter D | 0.8690 m              | 0.9561 m              |
| 4   | Liquid volume v   | 0.3865 m <sup>3</sup> | 0.5149 m <sup>3</sup> |
| 5   | Vessel pressure P | 101.3 kPa             | 101.3 kPa             |
| 6   | Height H          | 1.303 m               | 1.434 m               |

Fermenter for plant B sizing and specifications

**Table A7. Summary of pH adjuster specifications**

| S/N | Parameters        | A      | B                 |
|-----|-------------------|--------|-------------------|
|     |                   | Values | Values            |
| 2   | Vessel volume V   | -      | 50 m <sup>3</sup> |
| 3   | Vessel diameter D | -      | 3.488 m           |
| 4   | Liquid volume v   | -      | 25 m <sup>3</sup> |
| 5   | Vessel pressure P | -      | 101.3 kPa         |
| 6   | Height H          | -      | 5.232 m           |

Separator sizing and specifications for plants A and B

**Table A8. Summary of separator specifications**

| S/N | Parameters        | A                   | B                   |
|-----|-------------------|---------------------|---------------------|
|     |                   | Values              | Values              |
| 2   | Vessel volume V   | 2.00 m <sup>3</sup> | 2.00 m <sup>3</sup> |
| 3   | Vessel diameter D | 1.193 m             | 1.193 m             |
| 4   | Liquid volume v   | 1.00 m <sup>3</sup> | 1.00 m <sup>3</sup> |
| 5   | Vessel pressure P | 101.3 kPa           | 101.3 kPa           |
| 6   | Height H          | 1.789 m             | 1.789 m             |

Absorber sizing and specifications for plants A and B

**Table A9. Summary of absorber specifications**

| S/N | Parameters        | A                                       | B                                       |
|-----|-------------------|---|---|
|     |                   | Values                                  | Values                                  |
| 2   | Vessel volume V   | 8.836 * 10 <sup>-2</sup> m <sup>3</sup> | 8.836 * 10 <sup>-2</sup> m <sup>3</sup> |
| 3   | Vessel diameter D | 1.5 m                                   | 1.5 m                                   |
| 4   | Liquid volume v   | 101.3 kPa                               | 101.3 kPa                               |
| 5   | Vessel pressure P | 10.5 m                                  | 10.5 m                                  |
| 6   | Height H          | 0.5 m                                   | 0.5 m                                   |
| 7   | Tray spacing Ts   | 0.8836 m <sup>3</sup>                   | 0.8836 m <sup>3</sup>                   |
| 8   | Tray volume Tv    | 8.836 * 10 <sup>-2</sup> m <sup>3</sup> | 8.836 * 10 <sup>-2</sup> m <sup>3</sup> |

**Table A10. Summary of Absorber 2 specifications**

| S/N | Parameter         | A                             | B                             |
|-----|-------------------|-------------------------------|-------------------------------|
|     |                   | Values                        | Values                        |
| 2   | Vessel volume V   | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |
| 3   | Vessel diameter D | 1.5 m                         | 1.5 m                         |
| 4   | Liquid volume v   | 101.3 kPa                     | 101.3 kPa                     |
| 5   | Vessel pressure P | 10.5 m                        | 10.5 m                        |
| 6   | Height H          | 0.5 m                         | 0.5 m                         |
| 7   | Tray spacing Ts   | $0.8836 \text{ m}^3$          | $0.8836 \text{ m}^3$          |
| 8   | Tray volume Tv    | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |

Reflux absorber 1 sizing and specification for plant A and plant B

**Table A11. Summary of reflux absorber 1 specifications**

| S/N | Parameter         | A                             | B                             |
|-----|-------------------|-------------------------------|-------------------------------|
|     |                   | Values                        | Values                        |
| 2   | Vessel volume V   | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |
| 3   | Vessel diameter D | 1.5 m                         | 1.5 m                         |
| 4   | Liquid volume v   | 101.3 kPa                     | 101.3 kPa                     |
| 5   | Vessel pressure P | 10.5 m                        | 10.5 m                        |
| 6   | Height H          | 0.5 m                         | 0.5 m                         |
| 7   | Tray spacing Ts   | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |
| 8   | Tray volume Tv    | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |

Condenser sizing and specifications for plants A and B

**Table A12. Summary of condenser 1 specifications**

| S/N | Parameter         | A                             | B                             |
|-----|-------------------|-------------------------------|-------------------------------|
|     |                   | Values                        | Values                        |
| 1   | Vessel volume V   | $2.00 \text{ m}^3$            | $2.00 \text{ m}^3$            |
| 2   | Vessel diameter D | $1.00 \text{ m}^3$            | $1.00 \text{ m}^3$            |
| 3   | Liquid volume v   | 1.193 m                       | 1.193 m                       |
| 4   | Vessel pressure P | 101.3 kPa                     | 101.3 kPa                     |
| 5   | Height H          | 1.789 m                       | 1.789 m                       |
| 6   | Tray spacing      | $0.8836 \text{ m}^3$          | $0.8836 \text{ m}^3$          |
| 7   | Tray volume       | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |

Distillation sizing and specifications for plants A and B

**Table A13. Summary of distillation column specifications**

| S/N | Parameter         | A                             | B                             |
|-----|-------------------|-------------------------------|-------------------------------|
|     |                   | Values                        | Values                        |
| 1   | Vessel volume V   | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |
| 2   | Vessel diameter D | 1.5 m                         | 1.5 m                         |
| 3   | Liquid volume v   | 101.3 kPa                     | 101.3 kPa                     |
| 4   | Vessel pressure P | 10.5 m                        | 10.5 m                        |
| 5   | Height H          | 0.5 m                         | 0.5 m                         |
| 6   | Tray spacing      | $0.8836 \text{ m}^3$          | $0.8836 \text{ m}^3$          |
| 7   | Tray volume       | $8.836 * 10^{-2} \text{ m}^3$ | $8.836 * 10^{-2} \text{ m}^3$ |

Condenser sizing and specifications for plants A and B

**Table A14. Summary of condenser specifications**

| S/N | Parameter         | A                  | B                  |
|-----|-------------------|--------------------|--------------------|
|     |                   | Values             | Values             |
| 1   | Vessel volume V   | $2.00 \text{ m}^3$ | $2.00 \text{ m}^3$ |
| 2   | Vessel diameter D | $1.00 \text{ m}^3$ | $1.00 \text{ m}^3$ |
| 3   | Liquid volume v   | 1.193 m            | 1.193 m            |
| 4   | Vessel pressure P | 101.3 kPa          | 101.3 kPa          |
| 5   | Height H          | 1.789 m            | 1.789 m            |

Reboiler sizing and specifications for plants A and B

**Table A15. Summary of reboiler specifications**

| S/N | Parameter         | B                   |
|-----|-------------------|---------------------|
|     |                   | Values              |
| 1   | Vessel volume V   | 2.00 m <sup>3</sup> |
| 2   | Vessel diameter D | 1.00 m <sup>3</sup> |
| 3   | Liquid volume v   | 1.193 m             |
| 4   | Vessel pressure P | 101.3 kPa           |
| 5   | Height H          | 1.789 m             |
| 6   | Area              | 6.71                |

Cooler sizing and specifications for plant B

**Table A16. Summary of cooler specifications**

| S/N | Parameter | Cooler 1                     | Cooler 2                     |
|-----|-----------|------------------------------|------------------------------|
|     |           | Values                       | Values                       |
| 1   | Volume V  | 2.02 m <sup>3</sup>          | 2.46 m <sup>3</sup>          |
| 2   | Duty D    | 4.153 × 10 <sup>5</sup> kJ/h | 3.643 × 10 <sup>6</sup> kJ/h |
| 3   | Area A    | 7.6 m <sup>2</sup>           | 16.6 m <sup>2</sup>          |

Molecular sieve sizing and specifications for plants A and B

**Table A17. Summary of molecular sieve 1 specifications**

| S/N | Parameter                              | A      | B      |
|-----|--|--------|--------|
|     |  | Values | Values |
| 1   | Bottom pressure kPa                    | 101.3  | 1013   |
| 2   | Overhead pressure kPa                  | 101.3  | 1013   |
| 3   | Mass flow rate kg/h                    | 1086   | 1605   |
| 4   | Volumetric flow rate m <sup>3</sup> /h | 1.01   | 1.528  |
| 5   | Volume                                 | 3.03   | 4.584  |

**Table A18. Summary of molecular sieve 2 (plant B) specifications**

| S/N | Parameter                              | 2      |
|-----|--|--------|
|     |  | Values |
| 1   | Bottom pressure kPa                    | 100    |
| 2   | Overhead pressure kPa                  | 100    |
| 3   | Mass flow rate kg/h                    | 1650   |
| 4   | Volumetric flow rate m <sup>3</sup> /h | 1.556  |
| 5   | Volume                                 | 4.668  |

**Equipment Cost for all Plants**

**Cost Escalation**

All the cost-estimating methods use the historical data, and are themselves forecasts of the future costs. The prices of the materials of construction and the costs of labor are subject to inflation. Some methods have to be used to update old cost data for use in estimating the design stage and forecasting the plant's future construction cost. The method usually used to update the historical

cost data makes use of the published cost indices. These relate the present costs to the one-time costs, and are based on labor, material, and energy costs published in the government statistical digests.

$$\text{Cost in year A} = \text{Cost in year B} \frac{\text{Cost index in year A}}{\text{Cost index in year B}}$$

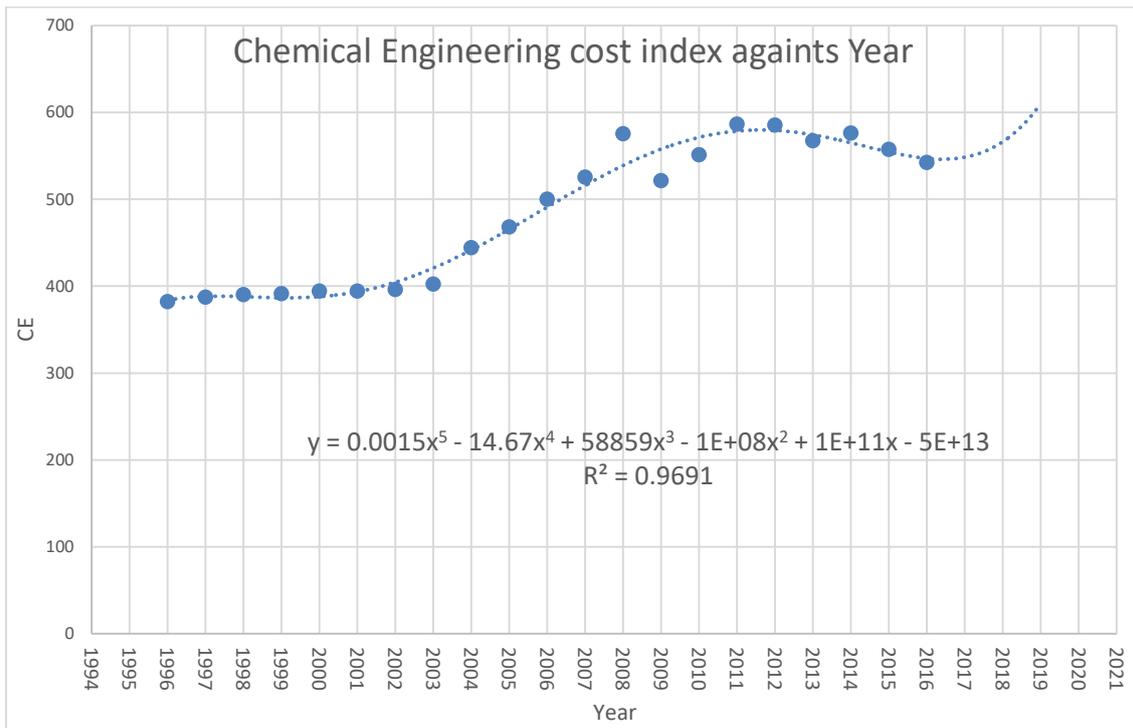


Figure B1. Graph of chemical engineering cost index against year

Table B1. Chemical engineering cost index for different years

| CE cost index | Year | Reference                  |
|---------------|------|----------------------------|
| 382           | 1996 | Richard <i>et al.</i> [32] |
| 387           | 1997 | Richard <i>et al.</i> [32] |
| 390           | 1998 | Richard <i>et al.</i> [32] |
| 391           | 1999 | Richard <i>et al.</i> [32] |
| 394           | 2000 | Richard <i>et al.</i> [32] |
| 394           | 2001 | Richard <i>et al.</i> [32] |
| 396           | 2002 | Richard <i>et al.</i> [32] |
| 402           | 2003 | Richard <i>et al.</i> [32] |
| 444           | 2004 | Richard <i>et al.</i> [32] |
| 468           | 2005 | Richard <i>et al.</i> [32] |
| 500           | 2006 | Richard <i>et al.</i> [32] |
| 525           | 2007 | Richard <i>et al.</i> [32] |
| 575           | 2008 | Richard <i>et al.</i> [32] |
| 521           | 2009 | Richard <i>et al.</i> [32] |
| 551           | 2010 | Richard <i>et al.</i> [32] |
| 586           | 2011 | Richard <i>et al.</i> [32] |
| 585           | 2012 | Richard <i>et al.</i> [32] |
| 567           | 2013 | Richard <i>et al.</i> [32] |
| 576           | 2014 | Richard <i>et al.</i> [32] |
| 557           | 2015 | Richard <i>et al.</i> [32] |
| 542           | 2016 | Richard <i>et al.</i> [32] |
| 550           | 2017 | Richard <i>et al.</i> [32] |
| 570           | 2018 | Extrapolation              |
| 610           | 2019 | Extrapolation              |

Table B2. Cost of a mixer for plant A

| Label | Type                      | V(ft <sup>3</sup> ) | V <sup>n</sup> | n   | C <sub>0</sub> | C <sub>n</sub> |
|-------|---------------------------|---------------------|----------------|-----|----------------|----------------|
| MX 1  | Kneader, sigma double arm | 131                 | 18.64          | 0.6 | 348594.5       | 375031.1       |
|       | Total                     |                     |                |     | 348594.5       | 375031.1       |

Source: Seider & Seader [29]

**Table B3. Cost of a mixer for plant B**

| Label | Type                      | $V(ft^3)$ | $V^n$ | n   | $C_0$    | $C_n$    |
|-------|---------------------------|-----------|-------|-----|----------|----------|
| MX 1  | Kneader, sigma double arm | 201       | 24.10 | 0.6 | 450790.5 | 484977.4 |
|       | Total                     |           |       |     | 450790.5 | 484977.4 |

Source: Seider & Seader [29]

**Table B4. Cost of a reactor for plant A**

| Label | Type               | $S(m^3)$ | A     | b     | n   | $S^n$ | $C_0$  | $C_n$    |
|-------|--------------------|----------|-------|-------|-----|-------|--------|----------|
| R1    | Jacketed, agitated | 2.0      | 14000 | 15400 | 0.7 | 1.62  | 38948  | 49828.6  |
| R2    | Jacketed, agitated | 72.7     | 14000 | 15400 | 0.7 | 20.09 | 323386 | 413727.9 |
| R2    | Jacketed, agitated | 0.5      | 14000 | 15400 | 0.7 | 0.62  | 23548  | 30126    |
|       | Total              |          |       |       |     |       | 385882 | 493682.5 |

Source: Sinnott [28]

**Table B5. Cost of a reactor for plant B**

| Label | Type               | $S(m^3)$ | A     | b     | n   | $S^n$ | $C_0$    | $C_n$    |
|-------|--------------------|----------|-------|-------|-----|-------|----------|----------|
| R1    | Jacketed, agitated | 1.146    | 14000 | 15400 | 0.7 | 1.62  | 30941.42 | 39585.3  |
| R2    | Jacketed, agitated | 3.5      | 14000 | 15400 | 0.7 | 20.09 | 51014.20 | 65265.7  |
| R3    | Jacketed, agitated | 1.03     | 14000 | 15400 | 0.7 | 0.62  | 27721.96 | 35466.4  |
| R4    | Jacketed, agitated | 3.488    | 14000 | 15400 | 0.7 | 0.62  | 50925.32 | 65151.9  |
|       | Total              |          |       |       |     |       | 160602.9 | 205469.3 |

Source: Sinnott [28]

**Table B6. Cost of a column for plant A**

| Label | Type       | S (m) | A   | b   | n | $S^n$ | $C_0$  | $C_n$  |
|-------|------------|-------|-----|-----|---|-------|--------|--------|
| DC1   | Sieve tray | 1.5   | 100 | 120 | 2 | 2.25  | 370    | 473.4  |
| AC1   | Sieve tray | 1.5   | 100 | 120 | 2 | 2.25  | 370    | 473.4  |
| AC2   | Sieve tray | 1.5   | 100 | 120 | 2 | 2.25  | 370    | 473.4  |
| RAC2  | Sieve tray | 1.2   | 100 | 120 | 2 | 1.44  | 272.8  | 349.0  |
|       | Total      |       |     |     |   |       | 1382.8 | 1769.2 |

Source: Sinnott [28]

**Table B7. Cost of a column for plant B**

| Label | Type       | S (m) | A   | b   | n | $S^n$ | $C_0$  | $C_n$  |
|-------|------------|-------|-----|-----|---|-------|--------|--------|
| DC1   | Sieve tray | 1.5   | 100 | 120 | 2 | 2.25  | 370    | 473.4  |
| AC1   | Sieve tray | 1.5   | 100 | 120 | 2 | 2.25  | 370    | 473.4  |
| AC2   | Sieve tray | 1.5   | 100 | 120 | 2 | 2.25  | 370    | 473.4  |
| RAC2  | Sieve tray | 1.2   | 100 | 120 | 2 | 1.44  | 272.8  | 349.0  |
|       | Total      |       |     |     |   |       | 1382.8 | 1769.2 |

Source: Sinnott [28]

**Table B8. Cost of a separator for plant A**

| Label | Type                   | S (kg) | a    | b   | n   | $S^n$  | $C_0$ | $C_n$   |
|-------|------------------------|--------|------|-----|-----|--------|-------|---------|
| S1    | Vertical, carbon steel | 15700  | -400 | 230 | 0.6 | 329.26 | 75329 | 96373.1 |
|       | Total                  |        |      |     |     |        | 75329 | 96373.1 |

Source: Sinnott [28]

**Table B9. Cost of a separator for plant B**

| Label | Type                   | S (kg) | a    | b   | n   | $S^n$  | $C_0$ | $C_n$   |
|-------|------------------------|--------|------|-----|-----|--------|-------|---------|
| S1    | Vertical, carbon steel | 15700  | -400 | 230 | 0.6 | 329.26 | 75329 | 96373.1 |
|       | Total                  |        |      |     |     |        | 75329 | 96373.1 |

Source: Sinnott [28]

**Table B10. Cost of a heater for plant A**

| Equipment | Type                  | $S(m^2)$ | a     | b    | n | $S^n$ | $C_0$ | $C_n$   |
|-----------|-----------------------|----------|-------|------|---|-------|-------|---------|
| HT1       | U-tube shell and tube | 10.5     | 10000 | 88   | 1 | 10.5  | 10924 | 13923.2 |
| HT2       | Double pipe           | 1.0      | 500   | 1100 | 1 | 1.0   | 1600  | 2039.3  |
|           | Total                 |          |       |      |   |       | 12525 | 15962.5 |

Source: Sinnott [28]

**Table B.11. Cost of a heater for plant B**

| Equipment | Type                  | S (m <sup>2</sup> ) | a     | b  | n | S <sup>n</sup> | C <sub>0</sub> | C <sub>n</sub> |
|-----------|-----------------------|---------------------|-------|----|---|----------------|----------------|----------------|
| HT2       | U-tube shell and tube | 13.9                | 10000 | 88 | 1 | 13.9           | 11223.2        | 14304.5        |
|           | Total                 |                     |       |    |   |                | 11223.2        | 14304.5        |

Source: Sinnott [28]

**Table B12. Cost of a cooler for plant B**

| Equipment | Type        | S (m <sup>2</sup> ) | a   | b    | n | S <sup>n</sup> | C <sub>0</sub> | C <sub>n</sub> |
|-----------|-------------|---------------------|-----|------|---|----------------|----------------|----------------|
| CL1       | Double pipe | 7.6                 | 500 | 1100 | 1 | 7.6            | 8860           | 11292.5        |
| CL2       | Double pipe | 16.6                | 500 | 1100 | 1 | 16.6           | 18760          | 23910.6        |
|           | Total       |                     |     |      |   |                | 27620          | 35203.1        |

Source: Sinnott [28]

**Table B13. Cost of a molecular sieve (modelled as a component splitter) for plant A**

| Equipment | Type            | S (m <sup>2</sup> ) | C <sub>0</sub> | C <sub>n</sub> |
|-----------|-----------------|---------------------|----------------|----------------|
| M1        | Molecular sieve | 3,03                | 257.55         | 277.1          |
|           | Total           |                     | 257.55         | 277.1          |

Source: Seider & Seader [29]

**Table B14. Cost of a molecular sieve (modelled as a component splitter) for plant B**

| Equipment | Type            | S (m <sup>3</sup> ) | C <sub>0</sub> | C <sub>n</sub> |
|-----------|-----------------|---------------------|----------------|----------------|
| M1        | Molecular sieve | 4.584               | 389.674        | 419.2          |
| M2        | Molecular sieve | 4.668               | 396.78         | 426.9          |
| M3        | Molecular sieve | 4.143               | 352.155        | 378.9          |
|           | Total           |                     | 1138.61        | 1225           |

Source: Seider & Seader [29]

**Table B15. Cost of a condenser for plant A**

| Equipment | Type          | S (lb/h.torr) | S <sup>0.41</sup> | n   | C <sub>0</sub> | C <sub>n</sub> |
|-----------|---------------|---------------|-------------------|-----|----------------|----------------|
| CD1       | Cooling water | 0.8859        | 0.9515            | 1.6 | 2915.40        | 3136.5         |
| CD2       | Cooling water | 0.9239        | 0.9681            | 1.6 | 2966.26        | 3191.2         |
|           | Total         |               |                   |     | 5911.66        | 6327.7         |

Source: Seider & Seader [29]

**Table B16. Cost of a condenser for plant B**

| Equipment | Type          | S (lb/h.torr) | S <sup>0.41</sup> | n   | C <sub>0</sub> | C <sub>n</sub> |
|-----------|---------------|---------------|-------------------|-----|----------------|----------------|
| CD1       | Cooling water | 0.8859        | 0.9515            | 1.6 | 2915.40        | 3136.5         |
| CD2       | Cooling water | 0.9239        | 0.9681            | 1.6 | 2966.26        | 3191.2         |
|           | Total         |               |                   |     | 5911.66        | 6327.7         |

Source: Seider & Seader [29]

**Table B17. Cost of a reboiler for plant A**

| Equipment | Type         | Q (million Btu/h) | C <sub>0</sub> | C <sub>n</sub> |
|-----------|--------------|-------------------|----------------|----------------|
| RB1       | Fired heater | 26.38             | 6996.28        | 7526.9         |
|           | Total        |                   | 6996.28        | 7526.9         |

Source: Seider & Seader [29]

**Table B18 Cost of a reboiler for plant B**

| Equipment | Type         | Q (million Btu/h) | C <sub>0</sub> | C <sub>n</sub> |
|-----------|--------------|-------------------|----------------|----------------|
| RB1       | Fired heater | 26.38             | 6996.28        | 7526.9         |
|           | Total        |                   | 6996.28        | 7526.9         |

Source: Seider & Seader [29]

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## 9. Conflicts of Interest

The authors declare no conflict of interests.

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