



Integrated Design of a Furfural Manufacturing Process from Bagasse

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ABSTRACT

Conservation of natural resources and pollution reduction are key elements in achieving sustainability. Furfural is one of the most promising sustainable platform chemicals for producing a variety of value-added products. Several studies have been published to optimize the performance of furfural plant design; however, this research introduces an innovative improvement in process integration. Both heat and mass integration strategies were investigated to enhance process efficiency, in addition to conducting an economic evaluation of the proposed plant. Simulation results using Aspen Plus V11 demonstrate that applying mass integration conserves 45% of the total fresh resources while enhancing profitability by saving approximately 0.5 million USD annually. The synthesis of Heat Exchanger Networks (HENs) resulted in total utility savings of 0.02 million USD annually. The proposed plant for producing furfural from sugarcane bagasse is commercially attractive, with a total capital investment estimated at 29.05 million USD and a net present value (NPV) of 19.29 million USD. Overall, profitability metrics including rate of return, payback period, equivalent annual annuity, and NPV sensitivity analysis indicate the economic viability of the plant.

1. INTRODUCTION

Bioeconomy, which relies on renewable bio-based resources to produce chemicals and energy, is a vital factor in meeting society's demand in a sustainable manner. Biomass materials, such as agricultural crops, have attracted increasing scientific research and commercial interest as sustainable sources of fuels and high-value chemicals over the last decade. A new generation of biorefineries has been developed that utilizes the hemicellulose component of the biomass in a selective manner. The IEA Bioenergy Task 42 defines the biorefinery as: "the sustainable processing of biomass into a spectrum of bio-based products (food, feed, chemicals, materials) and bioenergy (biofuels, power and/or heat)" [1]. Cellulose, hemicellulose, lignin, and starch are the main building blocks of any biomass. Hemicellulose is the second most abundant plant material after cellulose. In acid conditions, this hemicellulose is hydrolyzed to produce xylose (pentose), which is subsequently dehydrated to yield furfural. Furfural can be deployed as a foundation

chemical to create a variety of value-added products. It might also be used as a building component for other promising transportation biofuels such as ethyl levulinate and dimethylfuran [2].

The emergence of oil as a widely available raw material to produce "oil-based" polymers has halted studies for the potential use of furfural in the production of plastics [3]. Moreover, furfural manufacturing even now relies on outdated and inefficient technologies. The high manufacturing costs, along with low productivity, have diminished their competitiveness with petroleum-based products. There is no synthetic route available for furfural production; therefore, furfural is produced exclusively from renewable biomass resources by acid-catalyzed dehydration of pentoses [4]. According to Mamman, Lee et al. research, acid hydrolysis has shown to be the most efficient and cost-effective pre-treatment so far [5]. This acid hydrolysis is usually conducted using liquid sulfuric acid which is corrosive and forms homogeneous phase with furfural. To overcome the challenges of separating the furfural from the homogenous catalyst, several studies

have investigated heterogeneous solid catalysis, such as silicates [6], [7], zeolite [8], [9], tin-loaded sulfonated diatomite [10], coal fly ash [11], and carbon-based acid catalysts [12]. Moreover, Chunguang Rong et. al. studied the feasibility of the dehydration of xylose to furfural in biphasic system under atmospheric pressure. Experimentally, the highest furfural selectivity was achieved around 83% using sulfuric acid as catalyst plus an inorganic salt (NaCl) as promoter [13]. Although solid acid offers several advantages, it is expensive, prone to deactivation and its manufacturing is extremely difficult.

Several authors have conducted numerous studies to develop and improve the performance of furfural plant process design. Lars Moen [14] has designed a biorefinery utilizing 81.1% of corn stover, which corresponds to 47% of the total energy content, to produce ethanol and furfural. D. van Benthem et. al. [4], developed a process capable of converting 1000 kt/y bagasse into 65 kt/y of furfural in 98 wt.% purity with 100 kt/y of levulinic acid, 40 kt/y of formic acid. Additionally, it has also been proven that wheat straw, as a raw material, is economically and environmentally viable to produce furfural through combined dilute acid pretreatment of formic acid. Additionally, it has also been proven that wheat straw, as a raw material, is economically and environmentally viable to produce furfural through combined dilute acid pretreatment and thermally coupled distillation [15]. Wiebren De Jong et. al, have proposed a novel integrated 10 kt/y furfural production plant to improve the economic feasibility of the process [16]. A comparative study between distillation method against an innovative absorption method for purification of the furfural to achieve 99.8 wt.% purity and pure 5-methyl furfural, has been reported by G.S. Andrews et al [3].

Nowadays, industries place a high priority on reducing pollution, saving resources, boosting production, and maximizing profitability. Biorefineries have been criticized for using tremendous amounts of water and land resources [17]. According to several studies, process integration of biorefinery plants has the potential to boost production yields while reducing energy use [18] [19]. Process integration is a holistic approach to process design, retrofitting, and operation that emphasizes the unity of the process [20]. Hussain et al. [21] reported significant profitability of an integrated heat and mass system for furfural and glucose production from empty fruit bunches. Furthermore, an integrated plant that produces furfural, levulinic acid, and formic acid from oil palm empty fruit bunches was suggested by Denia Apriliani et al. [22] as having techno-economic viability. Substantial amounts of xylose are present in agricultural residues such as corn stover and sugarcane bagasse. Therefore, when low-cost residues can be used as raw materials, enhancements are economically realized. Bagasse is the remaining fiber after extracting the juice from crushed sugar cane. Sugar factories in Sudan produces which is usually burned around 1,060 kt of bagasse as a byproduct annually, to generate energy or used as fodder [23]. Thus, recently, interest has been realized in Sudan to exploit this wasted resource for more valuable products.

This paper delivers a performance evaluation and economic feasibility review of proposed plants to utilize this bagasse in sustainable and integrated design. The outcomes of this work will provide preliminary data for commercializing the implementation of the plant.

2. DESIGN METHOD

This study is part of a one-year project conducted in 2020 by the authors at University of Khartoum for sustainable design of furfural production plant in Sudan. The project was conducted through the following stages:

1. Degree of freedom analysis
2. Detailed material and energy balances
3. Process integration of mass and heat.
4. Process equipment design.
5. Utilities and ancillaries
6. Simulation verification
7. Process instrumentation and control.
8. Economic evaluation
9. Safety and loss prevention
10. Plant location and layout.

The scope of this paper will only cover the process modeling, and process integration of mass and heat. The process was simulated and analyzed using Aspen Plus V11.

3. PROCESS MODELING

The capacity to scale up to large output rates of furfural requires continuous process. Therefore, the Rosenlew process is considered the basis for the process design and improvement. The final piping and instrumentation diagram (P&ID) for the proposed plant is shown in figure 1:

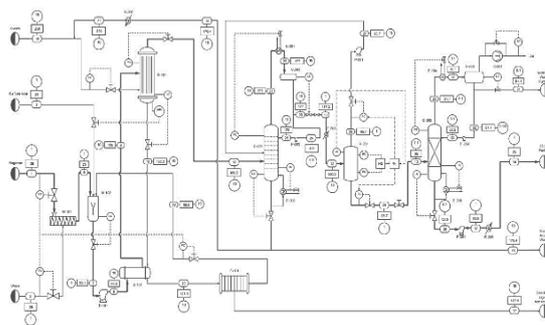


Figure 1. Furfural Plant P&ID Diagram [3]

The mixture ratio of the bagasse and water is an important criterion, because very low slurry density will require high steam consumption, and high density will result in clogging of the equipment. Practically, bagasse/water mass ratio of approximately 1:10 entering the reactor is technically feasible [16]. Dilute sulfuric acid (2.5 wt.%) is added, to catalyze the hydrolysis of pentosan and the dehydration of pentose to furfural. Moreover, the recycled filtrate is mixed for farther hydrolysis at atmospheric pressure. To have the highest yield of furfural, the optimum operating conditions of 10 bar and 180°C as

determined by the continuous process of Rosenlew were considered [23]. Therefore, pumping and heating are both applied. For heat integration purposes, the hot effluent sludge from the reactor is utilized to preheat the feed to the reactor. In the reactor, the overall reactions which also take place are:

$(C_5H_6O_{10})n \rightarrow (C_5H_4O_2)n$ + $2.H_2O$ (Desired reaction)	(1)
$C_5H_{10}O_5 \rightarrow C_5H_4O_2$ + $2.H_2O$ (Desired reaction)	(2)
$(C_6H_9Na_2O_{10}S_2)n \rightarrow (C_6H_7O_2)n$ (Undesired reaction)	(3)
$C_3H_6O_2 + H_2O \rightarrow C_2H_4O_2 + CH_3OH$ (Undesired reaction)	(4)

Besides these reactions, there are undesired irreversible resinification and condensation reactions that might occur for furfural. This is prevented by directly stripping furfural from the liquid phase through steam injection., 180°C and 10 bar, at the bottom. The distribution of the byproducts in the vapor and liquid phases are determined by their equilibrium concentrations under the operation conditions. The underflow of the reactor contains only 13 wt.% solids besides an abundance of water. Therefore, the effluent sludge from the reactor is delivered to a horizontal belt filter yielding a highly dewatered cake and a filtrate consisting essentially of water with small concentrations of sulfuric acid, xylose, arabinose and methyl pentosan. This filtrate is recycled for preparing feed stock slurry.

The water-furfural vapor-liquid equilibrium exhibits an azeotropic behavior. To purify the furfural to 99.5 wt%, reactor effluent enters the azeotropic distillation scheme. The bottom consists of water and some acids. The distillate, the water-furfural azeotrope, is condensed and sent to a decanter allowing for the liquid-liquid phase separation. To improve the separation efficiency of the decanter, a throttle valve is installed to reduce the pressure. The decanter pressure must be slightly higher than the atmospheric pressure to prevent leakage of air into the process, which can result in the polymerization of furfural. The water-rich phase in the decanter is sent back to the top of the column as part of the distillation reflux. Another column is used to separate the furfural product from the remaining water to maximize the quality of the product up to 99.5 wt% purity. The furfural-rich stream is fed to a vacuum distillation unit in which the bottom product is mainly furfural containing some 5-MF. The distillate is again the water-furfural azeotrope, which is sent back to the decanter. The distillation is done at vacuum conditions to ensure that the temperature never rises above 100°C, at which polymerization of furfural can occur [3].

4. MASS INTEGRATION

As sufficient details were available (e.g., flow sheet, mass balances and process models) a Mass Integration Targeting approach is used to benchmark the performance of the furfural manufacturing plant. According to El-

Halwagi [20] mass integration strategies for reaching the targets should follow the hierarchy:

1. No-/low-cost changes
2. Moderate cost modification
3. Innovative technologies

Mass-Exchange Integration for furfural plants of this scale is usually not very cost effective, because the costs of the additional equipment do not outweigh the benefits [3]. Therefore, only a direct recycling approach was considered. Direct recycling is the use of a processing stream (e.g., waste) in a process unit (i.e., a sink) without the addition of new equipment (no-/low-cost strategy).

Assumptions:

- Furfural and Methanol are the main impurities in all wastewater streams in this process. If furfural is considered for recycling to the mixer M-101, resinification and condensation reactions will occur. Therefore, this sink is excluded from direct recycling analysis to avoid any technical issues.
- The main purpose of filter F-201 is to integrate and keep the sulfuric acid inside the plant. Since reactor R-201 is the only sink available for sulfuric acid, the effluent of filter F-201 which has 30 wt.% solid content was excluded from the direct recycle analysis for two reasons. First, because it has resin polymers produced from the loss reactions. Second, to avoid the difficulties of matching its temperature with the reactor.
- Since furfural and methanol are the main impurities, the maximum inlet composition of the impurities to the reactor is considered as: the saturation concentration of furfural in steam that wouldn't condensed and starts the loss reactions. Moreover, to prevent any disruption in the decanter, methanol content should not distort the heterogeneous azeotropic curve.
- Water streams considered for recycling to the reactor should be heated to 179 °C to match the temperature of the reactor.

There are two process sinks that use fresh water: the mixer M-101 and the reactor R-201 (according to the first assumption, M-101 will be excluded). Three process streams (sources) are accessible for recycling: stream 31, 15 and 17 (according to the second assumption, stream 17 will be excluded). Before mass integration, a total of 10.8 kg/s of fresh water is used in both units, and a total of 19 kg/s of wastewater is discharged as effluent. It is desired to use direct recycling to reduce freshwater usage and wastewater discharge. As shown in Table 1, the following defines the parameters and constraints considered for the analysis.

To achieve the minimum usage of fresh streams, the lower bound of the acceptable flow rate for each sink is selected as the required flow rate. An optimization-based mathematical formulation for solving the direct recycling problem is presented as follows:

Objective: Minimize Fresh

Table 1. Sink and Source Data

Sink	Flow Rate [kg/s]	Maximum Inlet Mass Fraction [wt.%]	Maximum Inlet Load of Impurities [kg/s]
Reactor R-101	7.545	0.074	0.558

Source	Flow Rate [kg/s]	Mass Fraction [wt.%]	Load [kg/s]
31	0.069	0.36	0.025
15	7.087	0.02	0.155

The flow rate of the fresh is the sum of the flow rates of the fresh used in the process sink R-101, which is referred to as Fresh Steam. Therefore,

$$Fresh = Fresh_{Steam}$$

When considering direct recycling, the problem has two process sources (stream 15 and stream 31). Each of the process sources is split and fed to the process sink. Additionally, unrecycled process sources are discharged to the waste treatment system. The source-splitting constraint

$$Steam_{15} = steam_{15_to_Steam} + Steam_{15_to_Discharge}$$

Similarly, the splitting constraint for the effluent discharge source is given by:

$$Steam_{31} = steam_{31_to_Steam} + Steam_{31_to_Discharge}$$

Next, the mixing of the split sources and assigning them to sink is represented. The following is the flow and component balance constraints for the water and the pollutant entering the sink:

$$\begin{aligned} Fresh_{Steam} + Steam_{15_to_Steam} \\ + Steam_{31_to_Steam} &= 7.545 \\ Steam_{15_to_Steam} * 0.022 \\ + Steam_{31_to_Steam} * 0.3598 &< \\ &= 7.545 * 0.02 \end{aligned}$$

Similarly, the total flow rate going to waste treatment is given by:

$$Waste = Steam_{15_to_Discharged} + Steam_{31_to_Discharged}$$

Additional constraints are also required to ensure the non-negativity of the variables and the proper bounds on the feeding to the sink. This formulation was solved using LINGO programing.

5. HEAT INTEGRATION

HENs are common heat recovery systems in process industries developed by Linnhoff et. al. [24] to minimize utility costs. One of the most powerful aspects in synthesizing HENs is the identification of minimum utility targets ahead of designing the network. In this study, Aspen Plus V11 was used for HENs analysis.

This plant has four process hot streams (H11, H29, H37 and H21), three process cold streams (C15, C202 and C205), a heating utility (HU), and a cooling utility (CU). The data are given in Table 3. A value of $\Delta T_{min} = 10^{\circ}C$ is used. Using targeting techniques, it's desired to determine the minimum heating and cooling requirements. Also, develop an HEN implementation matching the hot and the cold streams to achieve the minimum utility targets.

Table 2. Streams Data for the Furfural Plant

Process Streams	Heat Capacity [kW/°C]	Supply T [°C]	Target T [°C]	Required Duty [kW]
H11 (Water)	2974.23	96.31	96	910.71
H21 (Steam)	19333.14	177.74	176.93	15618.63
H29 (Water)	433.02	80.67	81.17	216.51
H37 (Furfural)	0.69	143.31	25	81.65
HU (Steam)	----	286.85	246.85	14018.41
C15 (Steam)	21397.80	179.34	180	14018.41
C201 (Steam)	8635.50	179.09	179.34	2169.82
C202 (Furfural)	441.88	143.24	143.74	220.94
CU (Water)	----	16.85	26.85	14018.41

Practically, the integration of heat between the reboiler and the condenser causes difficulties for the distillation column to start up and control. Moreover, above the pinch, the hot utility and the condenser can provide the required duty of the reboiler. On the other hand, below the pinch, the cold utility and the reboiler can satisfy the duty of the condenser [25]. Therefore, regarding the distillation columns, streams H21, H29, C201 and C202 were excluded from the heat integration analysis. Minimum utility targets via the thermal pinch diagram (Graphical approach) were applied for the remaining streams.

6. RESULTS AND DISCUSSIONS

The results of this study are presented in two main parts: first, the potential prospects of the proposed process integration for both mass and heat, and second, the economic feasibility of the project is reviewed.

Prospects of the process integration

Mass integration

This study has successfully utilized 100% of Stream 18, and up to 98% of stream 15 in direct recycling to the reactor. The result of the direct recycling analysis is shown in Figure 2.

This integration resulted in a reduction of 64.4% of fresh water, 22.8% of fresh bagasse and 2.1% in waste effluents. It's estimated that this proposed mass integration would result in considerable financial savings of about half-a million USD annually as shown in Table 4.

Heat integration

Figure 3 depicts the graphical pinch diagram considered for the HENs analysis:

Since there is no horizontal overlap wherever the cold-composite-stream is moved downward or upward, no direct heat exchange between the process streams is achievable.

Therefore, due to this thermodynamic infeasibility, the integration of the utilities rather than the process streams was investigated using Aspen Plus V11. Generally, two approaches to energy recovery simulation are available in Aspen Plus V11: The first one is in contacting hot and cold streams in heat exchanger models (HeatX), and the second one is in interconnecting of heater and cooler models by heat streams. The following results were obtained from the Aspen Energy Analyzer (AEA):

- Minimum Heating= 16189 kW
- Minimum Cooling= 16172 kJ/h
- Number of heat exchange units= 10
- Total surface area for the heat exchangers= 343.7 m²

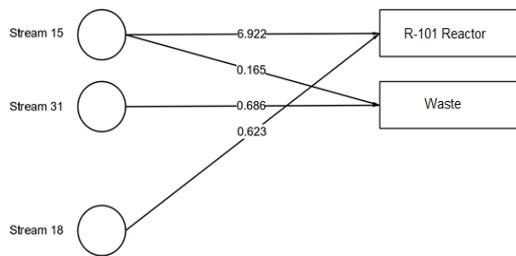


Figure 2. An implementation of the targets for the Furfural plant (all numbers represent assigned flow rate from source to sink in kg/s)

Table 3. Mass Integration Economic Benefits

Stream	Price [USD/kg]	Flow rate reduced [kg/s]	Cost savings [USD/year]
Stream 18 (MP Steam)	0.002	+ 6.922	+ 412,661.952
Stream 1 (Bagasse)	0.050	+ 2.056	+ 134,705.00
Streams 15 & 31 (Waste)	0.036	+ 0.165	+ 7805.16
Total			+ 555,172.112

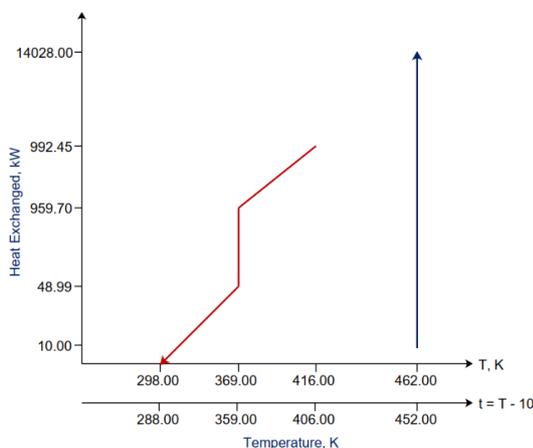


Figure 2. The thermal pinch diagram

This HEN analysis has resulted in considerable savings of about 0.028 million USD annually for the heating utility, and 0.007 million USD annually for the cooling utility

7. ECONOMIC EVALUATION

7.1 Capital and operating costs

To calculate the total process equipment cost, different methods were used. All equipment costs in the reaction section, as well as in the purification section, were calculated from data taken from Robin Smith [26]. The price increase over the years is considered by using the CECPI [27]. A concise summary of the resulting equipment costs is given in Table 5.

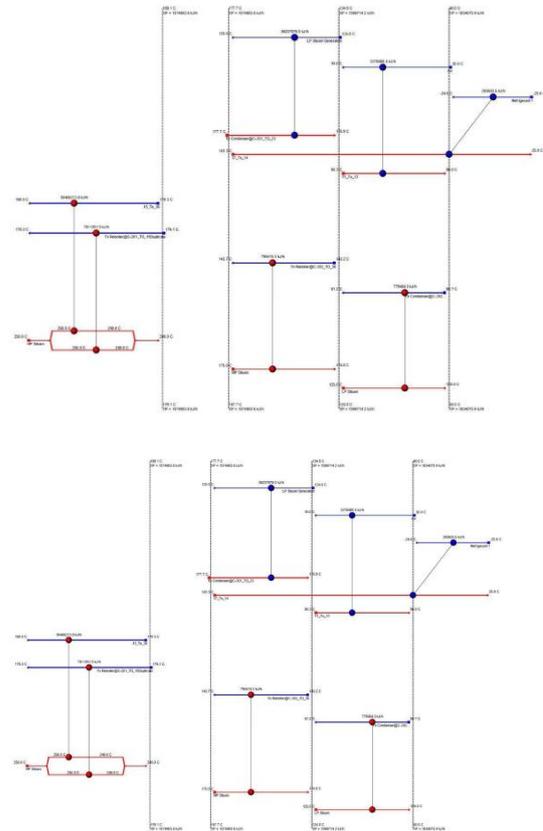


Figure 3. HEN intended to minimize total annualized cost

Table 1 Summary of the equipment and operating costs in million US dollars.

Process Equipment Cost (PEC)	Million USD
Reaction section	3.185
Purification section	1.918
Total	5.104

Operating Costs	Million USD/ yr	% APC
Direct Manufacturing Costs	16.519	79.59
Fixed Manufacturing Cost	4.567	6.86

General Manufacturing Expenses	2.971	13.55
Total Costs	24.057	100

7.2 Income

In the purification section, furfural is separated from the product stream very selectively. To reach the market specifications, furfural is separated and purified. It's assumed that furfural is the only product that can be sold in the market at a price of 2.38 USD/kg, therefore the total sales (Production-rate 1476 kg/hr) will be 29.23 million USD/y.

The cash flow, Figure 6, is attained from the difference between the income minus operating cost, taking into consideration the TCI, working capital, land and the salvage value of the equipment. It's assumed that this project will have an economic lifetime of 12 years.

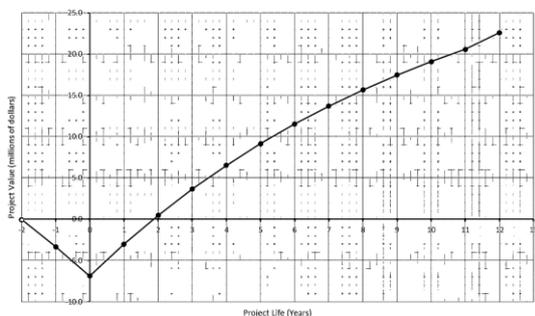


Figure 4. Cash Flow

7.3 Profitability Metrics

A discounted rate of return is an average rate of return calculated by expressing average annual profit as a percentage of the average value of the investment.

Discounted rate of return = 36.63%

Discounted Payback Period: The discounted payback method overcomes the weaknesses of the payback period by discounting the cash flow of the project with the cost of capital for the business and calculating the payback period based on the present value of the cash flows.

- Discounted Payback Period = 1 Year and 8 months
- Net present value: The net present value the value obtained by discounting all the cash outflows and inflows of a capital investment project, at a chosen target rate of return or cost of capital.
- Net present value = \$19.29 million USD
- Equivalent annual annuity (Capitalized cost): It's used to compare the net present values on an annualized basis.
- Equivalent annual annuity = \$ 3.3154 million USD/y
- Sensitivity analysis: it assesses how sensitive the NPV of a project is to the changes in various inputs to the NPV model. For the furfural process considered, the sensitivity of annual revenue,

interest rate (i%), and FCI were determined with respect to the NPV.

Table 6. Sensitivity Analysis for the Furfural Plant (Figures are in Millions USD)

Parameter	Value			
+0.5%	NPV of +0.5%	Value of 0.5%	- NPV of -0.5%	Value of -0.5%
Revenue	4.514	19.268	4.347	18.329
FCI	5.799	18.763	5.741	18.834
i%	0.105	17.982	0.095	19.656

CONCLUSION

This paper demonstrated a novel sustainable design of furfural manufacturing plant to recover waste effluents of bagasse in sugar production plants in Sudan. To appraise the feasibility of the proposed design, process simulation and economical evaluations were conducted.

The economic evaluation reveals that at current prices, a total investment of 29.05 million USD is requisite to install the plant. Contingency fees and shipping costs have not been included in the economic analysis. The net-present value of this investment is 19.3 million USD with a payback period of 1 year and 8 months and IRR of 36.63%, which are apparently appealing. The sensitivity within ± 5% expected variation of annual revenue, interest rate (i%), and FCI were determined with respect to the NPV.

The integration of mass applied for this process will prevent pollution and disposal of waste (2.1% reduction), conserve resources (bagasse 22.8% saving, water 64.4% saving) and enhance profitability by saving 0.5 million USD annually. Synthesis of Heat Exchanger Networks (HENs) resulted in total utilities saving of 0.02 million USD annually.

This research confirms the technical viability of the process and demonstrates its economic attractiveness, and has a promising future on a large scale.

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