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Sugarcane Bagasse Valorization to Xylitol: Techno-economic and Life Cycle Assessment

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Abstract

A detailed techno-economic analysis (TEA) and life cycle assessment (LCA) of a novel bio-refinery that produces xylitol from sugarcane bagasse. The proposed process includes dilute acid pretreatment in pressurized condition followed by fermentation (upstream section). The fermentation broth is then sent for separation and purification to the downstream section. Calculations are performed for a plant with 4 t/h of dry bagasse throughput. With fermentation yield of 0.54 g xylitol per g of xylose, the plant produced 437.4 kg/h of xylitol. Upstream data are adapted from experimental studies, while ASPEN PLUS® flowsheet simulation is used to get data for the downstream section. The xylitol production facility is assumed to be annexed to an existing sugar mill in India. The total utility requirement in the process is reduced using heat integration strategies. Cradle-to-gate scope is considered for LCA and 1 kg of xylitol is taken as the functional unit. The product cost of xylitol is calculated to be 230 INR/kg ($ 3.17/kg). For a four year payback period, the selling price of xylitol must be 450 INR/kg ($ 6.2/kg). Fermentation and pretreatment sections are the major components of the product cost. LCA results show that life cycle greenhouse gas emissions are 2.759 kg CO_2 eq. per kg xylitol. Electricity requirement within the plant is identified as the major sources of greenhouse gas emissions, and reduction in fermentation duration is identified as a key factor. The results identify opportunities to improve the process from economic as well as environmental standpoint.

Keywords: Bagasse; Sustainability; India; Biochemicals; Circular bioeconomy

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1. Introduction

Biomass based resources, especially lignocellulosic resources such as agricultural residue and forestry residue, are abundantly available. Circular bioeconomy principles propose that these resources must be utilized for value retention or value creation as much as possible. However, much of the lignocellulosic residues are currently either not used at all, or are used in relatively low value applications such as heat. Principles of green engineering argue that embedded complexity in these materials must be viewed as an investment by nature and should be used to our advantage. From that standpoint, recovering chemicals for high value applications is a more appropriate circular bioeconomy route. The focus on producing biochemical is, therefore, being viewed as a promising and sustainable pathway for enabling circular bioeconomy.

Xylitol, a polyol, is identified as an important value-added chemical that can be produced from biomass.[1] Xylitol is used globally as a diabetic sweetener as well as in other sectors such as food industry, dental care, and pharmaceuticals.[2] The global annual production of xylitol in 2017 was 190,900 MT,[1] and it is projected to reach 266,500 MT by 2022. The average selling price of the xylitol in the market is $ 4.5 – 5.5/kg.[3]

Unlike many other chemicals, xylitol is produced from biomass resource and there is no fossil-based alternative. The most common route is catalytic hydrogenation of xylose, which requires severe reaction conditions (high temperature and pressure) for the catalytic hydrogenation of pure d-xylose solution.[4] This increases the cost and also makes xylitol production carbon intensive. Therefore, alternative routes that utilize milder conditions and provide reduction in carbon intensity are desirable. Biochemical route based on fermentation of xylose sugars using suitable microbes is a possible option.[5] Biochemical processes are generally performed at

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ambient pressure and require minimal temperature modifications. This means that the overall conditions are less severe. Moreover, biological processes are dependent on natural agents (microorganism).

The biochemical route starts with dilute acid hydrolysis (pretreatment), fermentation and finally purification and separation. Various experimental methods for xylitol production using various lignocellulosic biomass have been reviewed by Antunes et al.[6] They reviewed studies using various lignocellulosic feedstocks such as sugarcane (bagasse and straw), corn (cob, stover and straw), rice straw, wheat straw, and sunflower stalks. Canilla et al.[7] reported a xylitol yield of 0.9 g/g xylose obtained from wheat straw, while Ping et al.[8] reported a yield of 0.7 g/g xylose from corn cob. Their experiments were done using a batch fermentation unit with batch time of 84 hours. Both these studies used dilute acid hydrolysis as the pretreatment step to separate hemicellulose from the lignocellulosic biomass. The studies though have been performed at bench scale and it is possible that certain operational issues may arise during scale-up of the processes.

As mentioned previously, xylitol is produced from biomass, and such processes are often considered to sustainable due to the renewable nature of biomass. Moreover, biochemical processes are also considered to be more benign than purely chemical routes due to the use of milder operating conditions. However, this does not guarantee sustainability and a systematic assessment is necessary. Life cycle assessment (LCA) is a comprehensive approach that has been used to study various biochemical routes for chemical production and has provided information regarding emission hotspots as well as process improvement opportunities.[9,10] LCA has also been increasingly used on novel and emerging technologies to provide feedback at an early stage of process development. In addition to the environmental impacts, the economic feasibility must

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also be assessed since overall sustainability of the process also includes the economic dimension. This can ascertain whether the product produced using the new route can compete in the market with the one produced from an established route. Techno-economic assessment (TEA) is commonly used for early stage evaluation of scale-up potential of novel processes. It is also critical to perform the TEA and LCA studies simultaneously on the same process with same scope and assumptions. If these studies are done separately, the results can often not be compared directly.

Prabhu et al. [11] have proposed a process to convert five carbon sugars in sugarcane bagasse (xylose) to produce xylitol. It is envisioned that this process can be integrated with an existing sugar mill and can utilize excess bagasse available with the mill. In this process, bagasse is first subjected to dilute acid pretreatment to recover xylose, which is fermented to produce xylitol. Residue containing mainly cellulose and lignin can be used for separately for energy or product recovery. Laboratory scale studies have achieved good yields, and therefore, the process can be a candidate for commercialization and scale-up.

As mentioned previously, detailed TEA and LCA studies of new processes are essential. The novel contribution of this work is to perform detailed techno-economic and life cycle assessment of this process. The work provides information regarding its commercial feasibility and also identify process improvement opportunities. By performing these studies together, the results can quantify the trade-offs, if any, between the different dimensions of sustainability can be determined. The methodology used here seamlessly integrates experimental data available from multiple sources with detailed flowsheet simulations. This results in highly reliable estimates.

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This is also the first such study done in the Indian context, where management of sugarcane bagasse is an important challenge requiring sustainable solutions.

The next section provides a detailed description of the proposed process. The TEA and LCA methodology are explained in the following section, and includes details pertaining to the flow sheet simulation and life cycle calculations. Subsequently, important results and impact of various operating parameters are discussed through multiple scenarios. The important conclusions are summarized in the final section.

2. Process Description

The process (Figures 1 and 2) has been split two sections, namely, upstream and downstream sections. It is assumed that bagasse with 35% moisture content is fed to a size reduction device such as hammer mill. This is followed by the pretreatment process developed by the Nova Pangaea Technology Limited. In the pretreatment reactor, bagasse undergoes dilute acid pretreatment using dilute sulfuric acid with steam at 11 bar (g) pressure. The required concentration of sulfuric acid is obtained by using 60 l of 98% sulfuric acid. The residence time for the pretreatment process is 15 minutes, and the temperature is maintained at 170 °C. Water and acid (raw material) are the inputs to the reactor, and electricity is required for agitation. Pretreatment depolymerizes xylan in hemicellulose to xylose, and cellulose and lignin mostly remain in the solid residue. The output of this pretreatment reactor is at high pressure, and a flash vessel is used to separate the waste water and toxins. The toxins are mainly organic acids (e.g., pyruvic acid) that are potentially harmful to the bacterium used in the fermentation step. The product stream from the flash vessel is sent to a water washing unit (washer) followed by screw press for squeezing out water. In these units, xylose in liquid form is separated from the solid

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residue. All these stages utilize a significant amount of electricity. The liquid stream after pretreatment and washing stages containing xylose is sent for fermentation. Depending on the input concentration requirements in the fermenter, an additional step of evaporation or membrane separation can be added.

The xylose thus obtained is converted to xylitol using *Y. lipolytica PSA02004* in a batch fermenter. The oleaginous yeast *Y. lipolytica* cannot grow on xylose as sole carbon source but can transform it to xylitol. Therefore, glycerol is used as co-substrate for cell growth. The cell biomass accumulated on glycerol transforms xylose into xylitol. Since xylose metabolism cannot go beyond xylitol, there is no possibility of side product formation. Moreover, high conversion efficiency of xylose to xylitol (92-97%) also rules out any by-product formation. The starting pH is 6.8 and not controlled during fermentation as *Y. lipolytica* is naturally adapted to grow efficiently even under low pH (<4.0). Xylitol production is observed to be unaffected with drop in pH. The process has been optimized as follows. The work involved screening of primary carbon source (glucose and glycerol), media optimisation in shake flask, scale up in bioreactor and downstream processing of accumulated xylitol. The media composition was optimized with two-step medium optimization involving central composite design and artificial neural network coupled with genetic algorithm. The yeast amassed 53.2 g/L of xylitol during batch cultivation in bioreactor using optimized media composition with a bioconversion yield of 0.97 g/g. Similar results were obtained when pure glycerol was substituted with crude glycerol from biodiesel industry (titer: 50.5 g/L; yield: 0.92 g/g).

The fermenter is operated at a temperature of 37 °C and a pH of 7.5, while the residence time in the fermenter is 168 hours. Use of sulfuric acid in the pretreatment stage leads to a reduction of the pH. This is addressed by adding $Ca(OH)_2$ (calcium hydroxide) so as to maintain the desired

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pH. $CaSO_4$ is produced as a byproduct due to the addition of calcium hydroxide. The fermentation output consists of $CaSO_4$ in solid phase with xylitol mixed with unconverted xylose and water in the liquid phase. The two phases are separated using a filtration unit, and the liquid stream containing xylitol is the fed to an adsorption unit to remove impurities using the activated carbon as the adsorbent. Subsequently, the stream containing xylitol enters the downstream unit for separation and purification.

The feed to the downstream section contains 7.65 % (by weight) xylitol and 92.35 % (by weight) water. The downstream separation starts with a quadruple-effect evaporative system that concentrates xylitol to 46.4 % (by weight). After concentrating, the solution is mixed with ethanol (75% by weight) and is fed to a crystallizer unit that operates at -5°C. Ethanol acts as an anti-solvent and reduces the solubility of xylitol in ethanol-water as the temperature decreases. Consequently, xylitol crystallizes out in this step. The addition of ethanol also lowers the freezing point of the solution. The output crystallizer is fed to a filtration unit which separates xylitol crystals from the ethanol-water mixture. The ethanol-water is mixture is fed to a distillation unit and after distillation, the ethanol is recycled back to the mixing unit. Solid xylitol obtained from the filtration still contains some moisture, and therefore, is sent to a counter-current dryer unit in which hot air is used to remove the residual moisture. The dried xylitol crystals are cooled down to ambient temperature and packed.

3. Process scale-up and flowsheet development

Considering the process previously described, a flow sheet for an industrial scale plant that processes 4 dry tonnes/hr of bagasse, thereby producing 3,464 tonnes of xylitol per year, has been developed. The experimental results for the pretreatment stage are reported for this throughput. Therefore, process performance and equipment cost data can be directly adapted for

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the TEA calculations. The process data for the upstream section of pretreatment and fermentation are adapted from experimental studies already reported in literature. The filtration unit after fermentation is considered to be a standard solid-liquid separator used after similar fermentation operations. The adsorption column is not rigorously modeled since adsorption isotherm data for the impurities could not be obtained. Instead, it is assumed that impurities are removed after the fermentation liquid is passed through the column. The capital and operating costs of filtration and adsorption units are calculated based on the flowrates, and these costs are added in the total cost calculation.

Experiments have not been performed for the downstream section. Therefore, ASPEN Plus® flow simulation is used to perform the material and energy balances and to determine the equipment sizes (Figure S1 in Supplementary Information). Table S1 in Supplementary Information shows the detailed process data. The NRTL (Non-Random Two Liquid) thermodynamic model is used in ASPEN Plus® flowsheet. The evaporator is modeled using flash and heater model in ASPEN Plus®.[12] The evaporator system has an overall steam economy and steam generation capacity of 2.81 and 4773.53 kg/h, respectively. Four effects in the multiple effect evaporator are finalized based on simulation trials and give the best steam efficiency. The saturation temperatures and pressures are adjusted so that the temperature difference between each effect is 15°C. In the first effect, the temperature is 90°C, while in the last effect it is 46°C. The crystallizer is modeled using the solubility data (mass of solute to mass of solution) for xylitol in ethanol-water mixture. It is assumed that the solubility of xylitol in ethanol-water is 0.5 at 30 °C and 0 at -5 °C.[13,14] Moreover, it is assumed that the residence time of crystallizer is 72 hours. The standard crystallizer module in ASPEN Plus® is used, which assumes that the cooling duty is provided by a refrigerant system operated using electricity. The filtration after crystallizer

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operates at atmospheric pressure conditions. The distillation column and filtration are modeled directly using the RADFRAC model and the filter model, respectively, in ASPEN Plus®. The distillation column is operated under atmospheric pressure. The column has 30 stages, reflux ratio of 4, and the top stage temperature in the column is 100 °C. The counter-current dryer unit is modeled using the counter-current heat-exchanger model in ASPEN Plus®, in which hot air is used. The air is assumed to be once through and not recirculated, with the inlet and outlet temperatures of 140 °C and 50 °C, respectively. The Xylitol outlet temperature at the outlet of the dryer was 102 °C.

As mentioned previously, this work assumes that the facility is annexed to a sugar mill providing sugarcane bagasse. The sugar mill will have a combined heat and power (CHP) unit providing steam. Moreover, medium to large scale mills in India have cogeneration plants producing electricity using excess bagasse. Based on this, steam and electricity are assumed to be available from the existing sugar mill. It also assumed that the cooling water will be sent to a cooling tower already set-up in the sugar mill. After the development of the basic flowsheet, the total steam requirement is reduced through heat integration. The process requires steam in the pretreatment reactors, first stage of the multiple effect evaporator, and distillation column to recover ethanol. The pretreatment reactor is fed with steam from medium pressure (MP) steam from the boiler as per the requirement. Similarly, the first effect of the evaporator is also fed MP steam directly from the boiler. The steam requirement for the distillation column though is met partly with steam from boiler and partly from internal heat integration. The vapor from the last of quadruple effect evaporator system has a temperature and a pressure of 46 °C and 0.096 bar, respectively. It is fed to three-stage compression unit to obtain a steam at 150 °C saturation temperature and 4.75 bar saturation pressure. This steam, with additional amount from the boiler,

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are used to met the steam requirement in the distillation column. The steam for the first effect of evaporator and pretreatment reactor is returned to the boiler, and it is assumed that 5% steam/water is lost requiring that make-up boiler feed water. The air preheater is assumed to be electric. The mass flow rates for the cooling water for the heat exchangers and condensers have been determined from ASPEN Plus® utility option. Cooling water is assumed to be available at 30 °C. The water loss in cooling tower 6% due to evaporation and blowdown. The boiler is fed with the solid residue from the pretreatment reactor, which contains cellulose, glucose and lignin. The solid residue is considered to have a calorific value of 14.08 MJ/kg and is completely sent to the CHP unit for steam and electricity generation. Overall energy balance shows that the total heat content of the residue is higher than the energy required to provide the necessary amount of steam after considering boiler efficiency of 0.9. In fact, there is a potential to generate extra steam than necessary. However, potential revenue from additional steam is not considered in this work.

4. TEA and LCA methodology

The methodology adapted to perform techno-economic and life cycle assessment is explained in this section. Figure 3 summarized the methodology starting from the process development stage.

4.1. TEA methodology

This work performs basic engineering design calculations that are typically subject to ±25% variability. We have used the methodology proposed by Towler and Sinnott.[15] for performing the TEA calculations. As per the method, the equipment cost first needs to be estimated, and the total capital investment is a function of the equipment cost. Since the pretreatment experiments were done for the capacity considered here, the equipment costs incurred by Nova Pangaea

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Technology are directly used. This includes the cost of pretreatment, flash vessel, washer, and screw press. Fermentation is performed in batch mode but the downstream process needs to operate on a continuous basis. Therefore, considering the fermentation residence time of 168 hours, seven fermenters are required. Each fermenter is assumed to have the liquid volume of 152.9 m^3 as per the volumetric flow rate of the liquid feed. The total volume of the fermenter is fixed assuming 10% additional head space. The costs of fermenter units are based on the study reported by Davis et al.[16] The costs are adjusted from the original source to match the capacity considered in this work as well as to account for the year of the analysis. Compressors are required for each fermenter to provide air for aeration. The size of the compressor is determine based on the aeration requirement, and the electricity requirement is estimated based on the standard compressor design calculations. The cost for adsorption columns is based on the cost reported in Mountraki et al.[17] The equipment costs of the downstream section are determined either from ASPEN Plus economic analyzer or from the website www.Matche.com.[18] Specifically, costs for heat exchangers, evaporators, chiller, and filtration unit are taken from the website. The costs of the cooling tower and CHP unit are not considered since the existing sugar mill is assumed to have already set it up.

The costs reported in Euros and USD have been converted to Indian Rupees (INR) assuming the currency conversion of INR 85 and INR 75, respectively. ASPEN Plus® provided equipment costs for 2016, and they have been converted to 2019 using the chemical engineering plant cost index (CEPCI). The labor and therefore fabrication costs of equipment in India is often lower than the global average. Therefore, the equipment costs reported by ASPEN Plus® or based fabrication data in UK or US are further reduced 30%.

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Based on the equipment cost, the procurement cost is calculated as 15% of the equipment cost. Further, the procured cost of equipment at the plat site is 40% of the fixed capital investment (FCI), which gives the total FCI. Working capital is 15% of the FCI. The total capital investment (TCI) is sum of the FCI and working capital. The calculation of TCI explained here is based on the practice followed by engineering design companies for projects in India.

The operating cost is calculated based on the methodology provided by Towler and Sinnott.[15] The raw material costs (Table S2 in Supplementary Information) are adapted from www.indiamart.com.[19] Since raw materials will often be purchased in bulk, the actual costs could be lower than those considered here. The utility includes the cooling water, boiler feed water, and process water. All the electricity and steam requirement for pretreatment unit as well as for the first effect of the quadruple-effect evaporator are met by using the CHP unit in the sugar mill. The steam required in the downstream units is provided by the effect of the quadruple-effect evaporator after feeding it to a three-stage compression unit. The electricity is available at 6 INR/kWh ($ 0.08/kWh), and cost of the boiler feed water is 90 INR/m^3 ($ 1.2/m^3).[20] The process water and cooling water cost is assumed to be 20 INR/m^3 ($ 0.27 /m^3). The recycling percentages for process, boiler, and cooling water are 10%, 5%, and 6%, respectively. The aeration rate for the fermenters is 1 liter per minute for 1 liter of fermentation liquid (1 vvm). By using this information, the electricity requirement for compressors is estimated. The total economic life and number of working days in a year for the plant are 10 and 330, respectively.

In the TEA, two scenarios are considered based on the cost of raw material (bagasse) and electricity. These two scenarios capture two possibilities of setting up a bagasse to xylitol plant, namely, a plant attached to an existing sugar mill, and a stand-alone plant set-up separately. If

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the plant is attached to an existing sugar mill, sugarcane bagasse will be available free of cost since it will be generated during sugarcane crushing. Additionally, most medium to large scale sugar mills in India generate electricity using excess bagasse, and excess electricity is sent to the grid. Therefore, electricity can also potentially be available free of charge. Therefore, in the first scenario (Scenario 1), bagasse and electricity are considered to be free for the proposed plant. In contrast, if the plant is set-up separately, bagasse and electricity will need to be purchased. Therefore, the second scenario (Scenario 2) assumes that the proposed plant has to purchase both bagasse and electricity. A comparison of the TEA results provides more insights regarding the scale-up options of this process.

4.2. LCA methodology

The goal of this study is to determine the life cycle impacts of xylitol production from sugarcane bagasse. The results will be compared with the impacts of other processes proposed in literature, and will also be useful for process developers for improving the process. The study can also be used to quantify the advantage of producing xylitol using the proposed as compared to the other route of catalytic hydrogenation. This is a cradle-to-gate LCA study and considers the farming, bagasse transportation, and the biorefinery processing stages (Figure 4). The functional unit is 1 kg of xylitol.

For determining the reference flows, the experimental data for processing of 4 dry tonnes/h of bagasse in combination with process simulation data for the downstream section are used. The data are scaled for 1 kg of xylitol as per the recommended practice. Table 1 shows the reference flows and their values, respectively.

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The life cycle inventory data for chemicals used in the process are obtained from the Ecoinvent® database (version 3.3). The database is also used to get inventory data for activated carbon and electricity. Since India specific data for electricity produced from biomass is available, it is used in the calculations. For other inputs, inventory data for RoW (Rest of the World) are used. The LCA model is developed in OpenLCA version 1.10.2 is used along with Recipe (H) Midpoint impact assessment method. Since there are no by-products, all the impacts are allocated to xylitol.

5. Results and discussions

This section reports the techno-economic assessment results followed by discussion of the LCA results.

5.1 Techno-economic analysis results

Table 2 summarize the key results of the techno-economic assessment for the two scenarios. The product cost of xylitol is 237 INR/kg ($ 3.16 /kg) in Scenario 1 (free bagasse and electricity). Typically, investment decisions are made based on payback period and a payback period of four to six years is desirable. For the proposed process, payback period of four years is achieved if xylitol is sold at 450 INR/kg ($ 6.0 /kg). The selling price can be 375 INR/kg ($ 5 /kg) if the payback period is allowed to go up to seven years. It must be noted here that this is a factory gate price and not the price paid by consumers in the market. Further assessment of the cost breakdown reveals that capital cost is the main contributor to the product cost of xylitol. This agrees with the previously reported studies in TEA of xylitol. Steps such as acid hydrolysis, fermentation, and evaporation contribute majorly to the capital costs. For the proposed process, 54% of the total equipment cost is contributed by the upstream section (including the

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fermentation unit). The fermentation unit is the significant contributor to the equipment costs in the upstream unit due to requirement of 7 fermenter units and associated compressor units. This implies that if the fermentation time can be reduced, without much reduction in the yield, the cost of production can be reduced.

The distribution of the total product cost among the various stages for both scenarios is shown in Figure 5. For scenario 1, the fermentation section, which includes the fermenters and compressor units as well as the filtration equipment, contributes 36% of the total product cost. This is followed by evaporator and compressor unit (28%) and pretreatment and washing units (20%). The recycling of solvent (ethanol), process, cooling, and finally the boiler feed water (condensate) significantly reduces the operating cost.

For scenario 2, as expected, the product cost increases to 347 INR/kg ($ 4.62/kg) since the facility also has to pay for bagasse and electricity. The difference was only due to higher raw material and utility costs since there was no change in the equipment sizes and process stream flow rates. The selling price has to be 560 INR/kg ($ 7.46/kg) to get a four years payback period, and this is 46% higher as compared to scenario 1. Even though capital investment continues to be the major cost component in scenario 2, the operating costs (raw material and utility costs) also play a significant role. Overall the energy requirement in the plant is very high due to significant requirement of electricity in the upstream as well as downstream section. The total electricity demand is 2779 kW, and 72% of this total demand is for fermentation and filtration units. This is followed by demands for pretreatment and washing unit (8.5%) and the evaporation and compressor units (9.67%).

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A comparison with TEA studies in literature has been performed. A techno-economic study done by Mountraki et al.[17] compared the catalytic hydrogenation and biochemical (xylose fermentation) routes for xylitol production. Capital investment and raw material costs were higher for the biochemical route compared to the catalytic route. They concluded that rigorous heat integration techniques could reduce the operating costs significantly. A study on the valorization of brewers spent grains considered three scenarios of production of xylitol and xylo-oligosaccharides.[21] Sensitivity analysis showed that the cost of brewers spent grains had the largest effect on break-even price of xylitol. Gerbrandt [22] considered two routes of xylitol production, catalytic hydrogenation and fermentation. The study discussed cellulosic ethanol production facility which co-produces xylitol.

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Özüdoğru et al.[3] discussed a bio-refinery producing xylitol, citric acid, and glutamic acid that was set-up next to a sugarcane mill co-producing electricity. Three scenarios, namely, producing xylitol, citric acid, or glutamic acid along with co-generation of electricity in each case, were considered. For xylitol production scenario, capital cost was high relative to the operating cost. However, since the electricity requirement was high, the quantity of electricity sold was lesser as compared to other two scenarios. They reported a selling price of $ 3 /kg. Giuliano et al.[23] determined the selling price to be $ 3.5 /kg, and concluded that co-production of ethanol and xylitol was desirable. Ou et al.[24] performed techno-economic analysis of a sugarcane production facility co-producing xylitol and polyols, and determined variation in sugar price with production of xylitol and polyols. For feedstock processing capacity of 1500 MT/day, the selling price of xylitol was $ 2 /kg. The co-production of the xylitol in the facility increased the capital costs but the commercial value of the xylitol was able to contribute to the profits. The selling price for both scenarios considered in this work are higher compared to the values reported in literature. This could be due to the presence of co-products in the process, which reduced the per unit production cost of xylitol. Moreover, the yield of xylitol plays a significant role in determining the break-even cost of xylitol. For the same plant the higher the yield then higher would be the profit. Increase in profits can balance the capital costs, since capital costs is the major cost in the present study, can reduce the selling price.

The current selling price of xylitol is $ 4.5 – 5.5 /kg,[3] and selling price for scenario 1 falls within this range. However, scenario 2 is definitely not economically feasible. As noted previously, this comparison is only indicative since the post-production supply chain costs and profit margins have not been accounted for here.

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5.2 Life cycle assessment results

The LCA results (Table 3) show that the climate change impact is 1.807 kg CO_2 eq. per kg of xylitol, and fermentation and filtration units are responsible for 68% of this total impact (Figure 6). This is followed by contribution from other stages such as pretreatment section (18%), evaporation and compressor section (9.9%), and bagasse farming (3.4%) (Figure 6). The climate change impact for the fermentation and filtration stage is driven by two factors. First, electricity required to provide 1 vvm aeration is quite high, leading to a large contribution to climate change impact. The second factor is the use of lime for neutralizing H_2SO_4. Life cycle emissions of lime contribute noticeably to the total climate change impacts of this stage. In the downstream section, compressor units require electricity, and therefore, the climate change impacts increase. Here, it must be noted that we have assumed a bagasse-based CHP unit already installed in the sugar mill. Even though the electricity used is produced from bagasse in the sugar mill, it still has some climate impact. Electricity produced from such a unit is considered to have a GHG emission factor of 0.28 kg CO_2 eq. per kWh (Ecoinvent v 3.3). In contrast, the GHG emission factor is 1.23 kg CO_2 eq. per kWh for production mix in India (Ecoinvent v 3.3). Therefore, if typical electricity source in India is assumed, the total climate change impact will increase to 10.75 kg CO_2 eq. per kg of xylitol.

The other category of interest is water depletion, and that impact is 2.975 m^3 per kg of xylitol. Electricity demand is again majorly responsible for water depletion, because it has the water use intensity of 1.42 m^3 water per kWh (Ecoinvent 3.3 database). Electricity is also mostly responsible for the human toxicity and fossil depletion impact categories. The use of bagasse results in increased particulate matter emissions (0.005 kg PM_{10} per kg xylitol), which is consistent with earlier observations related to biomass combustion.

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LCA study on catalytic hydrogenation of xylose to produce xylitol using empty fruit bunch as the feedstock has been reported.[25] Dasgupta et al. [26] performed LCA of xylitol production from corn cobs using the fermentation route, and reported a climate change impact of 8.68 kg CO_2 per kg xylitol. The process configuration was very similar to the one considered here. They also reported that the climate change impacts were mainly due to the energy consumption at various stages in the process, namely, acid hydrolysis, fermentation, and evaporation. The significantly higher impact as compared to this study could be due to two reasons. First, Dasgupta et al. considered electrical energy for evaporation. In contrast, this work has considered steam-based evaporation since that is more common for commercial scale plants. The steam in our process is produced by burning cellulignin leading to biogenic emissions that are not considered for calculating the climate change impact (biogenic CO_2). Second, this work has assumed that the electricity consumed has been produced using excess bagasse in the sugar mill. As a result, emissions due to bagasse burning are biogenic and hence not considered. In contrast, Dasgupta et al. considered grid electricity was North India, which is produced mainly from fossil fuels (coal and natural gas). Since we are assuming that the xylitol production plant is annexed to an existing sugar mill, use of bagasse-based electricity is justified. These factors lead to much lower life cycle climate change impact for our process as compared to that studied by Dasgupta et al.

Hafyan et al.[25] reported the climate change impact for 1 kg of xylitol from empty fruit bunch by catalytic hydrogenation to be 3.83 kg CO_2 eq. 95% of the CO_2 emissions in this case were due to the heat requirement in the process. The study by DuPont on their xylitol (XIVIA^{TM}) showed a life cycle CO_2 emission as 3.59 kg CO_2 eq. per kg xylitol.[27,28] Since further break-up of the total impact was not reported, it was not possible to perform detailed comparison with our process. In the same study though, it has been reported that the production of corn cob-based xylitol

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production using catalytic hydrogenation resulted in a significantly higher impact of 38.6 kg CO_2 per kg xylitol.

A comparison with literature shows that the impacts calculated here are lower than those reported earlier. Even though the study shows values which are optimistic, actual numbers for emissions will be revealed only after commercialization of the process. The important factor in all these studies is the significant amount of energy requirement for the process. In the current process the electricity requirement is the major contributor to the GHG emissions. Therefore, there is a need to look into cleaner electricity production that will reduce the life cycle emissions. Similar to the economic results, reducing the number of fermenters by shortening the fermentation time, will reduce the electricity required for aeration. This will reduce the overall climate change impact of the process.

5.3 Sensitivity analysis

The dependence of economic feasibility and the life cycle impacts on some of the assumptions made previous has been quantified by performing sensitivity analysis. The previous calculations have shown that capital cost, particularly the cost of fermenters, is a key contributor to the total cost of production. Each fermenter also requires aeration, which increases not only the cost but also the climate change impact due to the electricity consumption. The number of fermenters is high due to the assumption of 168 hours of fermentation, which necessitates multiple fermenters operating in parallel. Hence, sensitivity analysis has been performed by assuming that the fermentation time is 96 hours. Yield is also a very important factor that affects the economic feasibility of any product. Therefore, the impact of higher yield on the cost of production has also been quantified.

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The reduction in fermentation time from 168 hours to 96 hours has significant impact on the plant profitability and the LCA impacts. The reduction in fermentation time to 96 hours reduces the number of fermenters to four. This reduces the capital costs. The product cost will reduce by 15.6% to Rs. 200 /kg as compared to the base case. For a payback period of four years, the selling price will need to be Rs. 380 /kg, a reduction of 15.5%. For LCA impacts, reduction in fermentation batch time reduces the life cycle climate change impact from 1.807 kg CO_2 eq. per kg Xylitol to 1.385 kg CO_2 eq. per kg Xylitol. This is due to the lower electricity requirements for the compressor units in the fermentation units.

For the sensitivity analysis with respect to xylitol yield, two yield values, namely 0.648 g/g and 0.78 g/g, in addition to the base case yield of 0.54 g/g have been considered. The results show that there is linear reduction in the product cost. The product cost for 0.648 g/g yield is Rs. 194 /kg, while that for 0.78 g/g is Rs. 159 /kg. It is to be noted that the capital costs are the major costs that has significant impact on the product costs. The equipment is the major cost in the capital costs. Based on the assumptions used in the sensitivity analysis, the increase in the yield leads to decrease in the downstream equipment costs and hence the capital costs. As the mass fraction of the xylitol increases in the feed to the downstream unit, the size of the quadruple evaporator system decreases and thereby reducing the capital costs.

6. Conclusion

The techno-economic and life cycle assessment of the process proposed to produce xylitol from sugarcane bagasse shows that the process can be a sustainable alternative. The economic assessment shows that a commercial plant can be economically feasible under the ideal conditions considered here. The upstream stage of dilute acid pretreatment and fermentation contribute largest to the total product cost, and hence process improvement strategies should be

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explored. In particular, reducing the energy requirement in the pretreatment and reducing the time of fermentation can make the greatest contributions towards cost reduction. The reduction in fermentation time, however, can alter the yield, and hence this is an important optimization problem to be explored. The economics are also dependent on the price at which bagasse and electricity are available. The life cycle assessment results show the climate change impacts to be better than those for the catalytic hydrogenation route. Moreover, most of the climate change impact is due to the fermentation stage. This again points towards further optimization of fermentation operation. This work can be extended further by considering the use of solid residue from pretreatment for producing value added chemicals as opposed to burning. The results of this study can also be included in the larger sugar mill refinery optimization problem.

Acknowledgments

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Table 1 : Detailed process inventory for the production of 1 kg of xylitol

S. No.	Input	Value	Output	Value
1	***Farming stage*** ***(Bagasse for the process)***			
	Electricity (kWh)	**0.018**	Bagasse (kg)	**9.145**
	Diesel (kg)	**0.003**	Nitrogen Oxides (kg)	**0.004**
	Water (kg)	**659**	Phosphorous runoff (kg)	**0.001**
	Nitrogen (kg)	**0.007**	NH_3 emissions (kg)	**0.0006**
	Phosphorous (kg)	**0.002**		
	Potassium (kg)	**0.002**		
	Farm yard Manure (kg)	**0.241**		
	Pesticides (kg)	**0.000**		
2	***Pretreatment Reactor***			
	Bagasse (kg)	**9.145**	Product Stream 1 (kg)	**19.052**
	Electricity (kWh)	**0.537**		
	Water (kg)	**0.329**		
	Sulfuric Acid (kg)	**0.134**		
3	***Flash Unit***			
	Electricity (kWh)	**0.052**	Product Stream 2 (kg)	**17.856**

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	Product Stream 1 (kg)	**19.052**	Condensate (kg)	**1.196**
4	***Washer Unit***			
	Electricity (kWh)	**0.37**	Product Stream 3 (kg)	**13.871**
	Water (kg)	**2.778**	Product Stream 4 (kg)	**14.38**
	Product Stream 2 (kg)	**19.289**		
5	***Screw Press Unit***			
	Electricity (kWh)	**0.15**	Xylose (kg)	**0.205**
	Product Stream 4 (kg)	**14.38**	Cellulignin (kg)	**7.087**
6	***Fermentation & Filtration Unit***			
	Electricity (kWh)	**3.398**	Product Stream 5 (kg)	**13.069**
	Product Stream 4 (kg)	**13.871**	Bag house Lime (kg)	**0.152**
	Lime (kg)	**0.258**	Gypsum (kg)	**0.191**
7	***Adsorption Unit***			
	Product Stream 5 (kg)	**13.069**	Product Stream 6 (kg)	**13.069**
	Electricity (kWh)	**0.002**		
	Activated Carbon (kg)	**0.000**		
8	***Evaporator & Compressor Unit***			
	Product Stream 6 (kg)	**13.069**	Product Stream 7 (kg)	**2.165**
	Electricity (kWh)	**0.615**		
9	***Crystallizer & Filtration Unit***			

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	Product Stream 7 (kg)	**2.165**	Product Stream 8 (kg)	**1.000**
	Electricity (kWh)	**0.002**	Product Stream 9 (kg)	**3.969**
	Ethanol Stream (kg)	**2.804**		
10	***Ethanol Recovery Unit***			
	Product Stream 9 (kg)	**3.969**	Xylitol Stream (kg)	**1.000**
	Electricity (kWh)	**0.0025**	Ethanol Stream (kg)	**2.804**
11	***Drying & Cooling Unit***			
	Xylitol Stream (kg)	**1.000**	Xylitol (kg)	**1.000**
	Electricity (kWh)	**0.028**		

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Table 2 : Results of techno-economy assessment of xylitol production from sugarcane bagasse for scenario 1 (with bagasse and electricity free) and scenario 2 (with bagasse and electricity not free)

Parameter	**Scenario 1 (bagasse and electricity free)**	**Scenario 2 (bagasse and electricity not free)**
Product cost (INR/kg)	237 ($ 3.16 /kg)	347 ($ 4.62 /kg)
Selling price for four-year payback period (INR/Kg)	450 ($ 6 /kg)	560 ($ 7.46 /kg)
NPV (Million INR)	1,281	1,286
Raw material cost (Million INR)	40	167
Utilities cost (Million INR)	4.25	136
Purchased equipment cost (Million INR)	943	943

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Table 3: Life cycle impacts for production of 1 kg of xylitol for important impact categories

Impact category	**Overall impacts for the process**
Climate Change (kg CO_2 eq)	1.807
Fossil depletion (kg oil eq)	0.184
Freshwater ecotoxicity (kg 1,4-DB eq)	0.016
Human toxicity (kg 1,4-DB eq)	0.558
Particulate matter formation (kg PM_{10} eq)	0.006
Photochemical oxidant formation (kg NMVOC)	0.018
Water depletion (m^3)	2.795

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List of figures and figure captions

Figure 1: Upstream section for xylitol production process including pretreatment, separation and fermentation

Figure 2: Downstream section for xylitol production process including adsorption, evaporation, crystallization, and ethanol separation

Figure 3: Methodology adapted to perform techno-economic and life cycle assessment of the proposed process

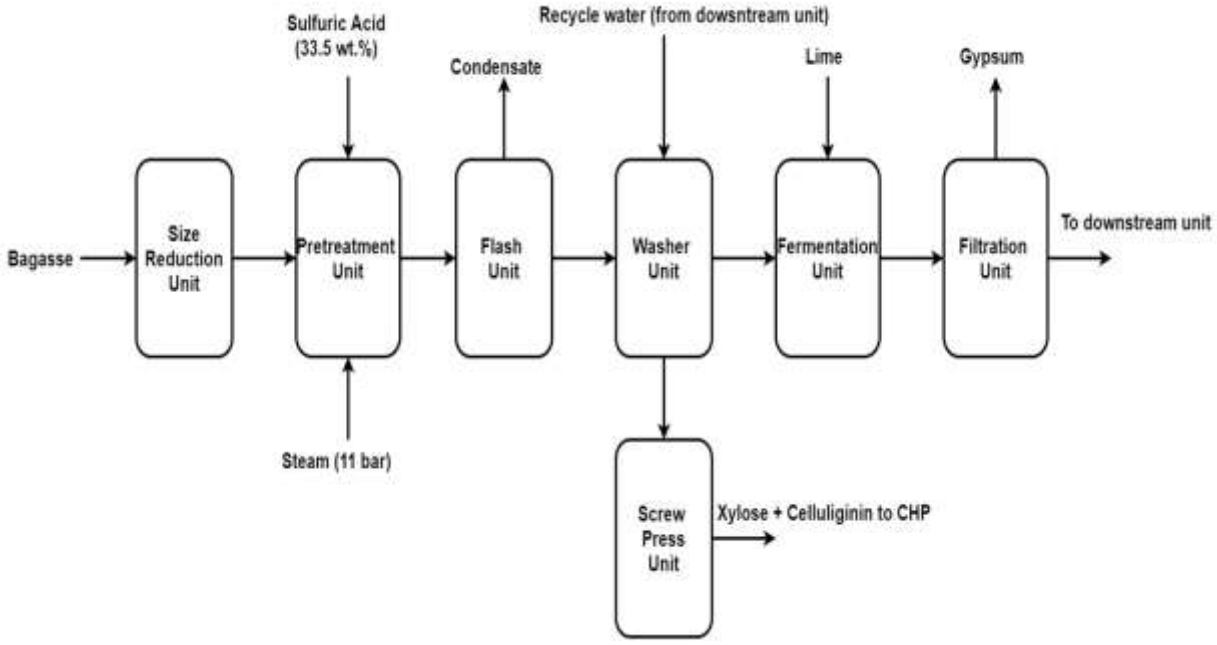
Figure 4: System boundary and product system for the xylitol production process

Figure 5: Contribution of various production and processing stages to the total xylitol product cost for scenario 1 (with bagasse and electricity free) and scenario 2 (with bagasse and electricity not free)

Figure 6: Contribution of different production and processing stages to the total climate change impact for 1 kg of xylitol

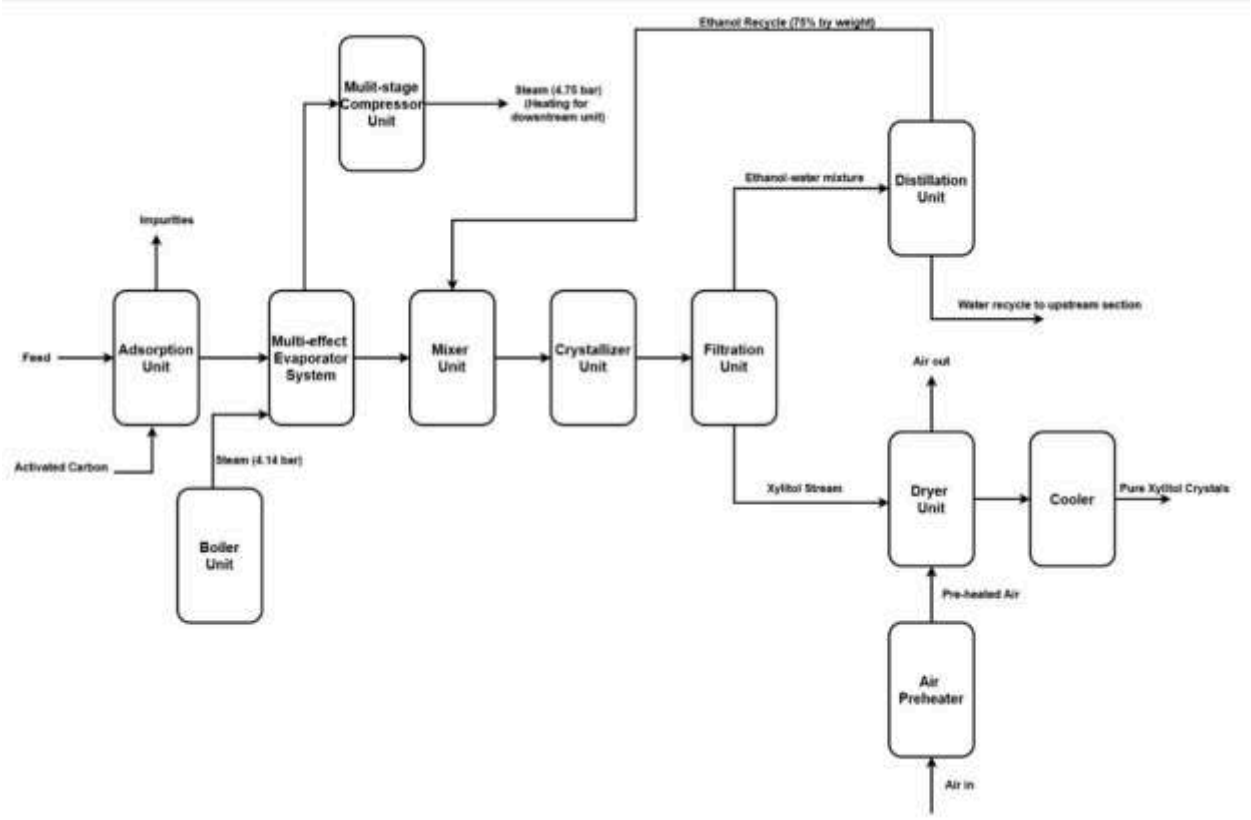
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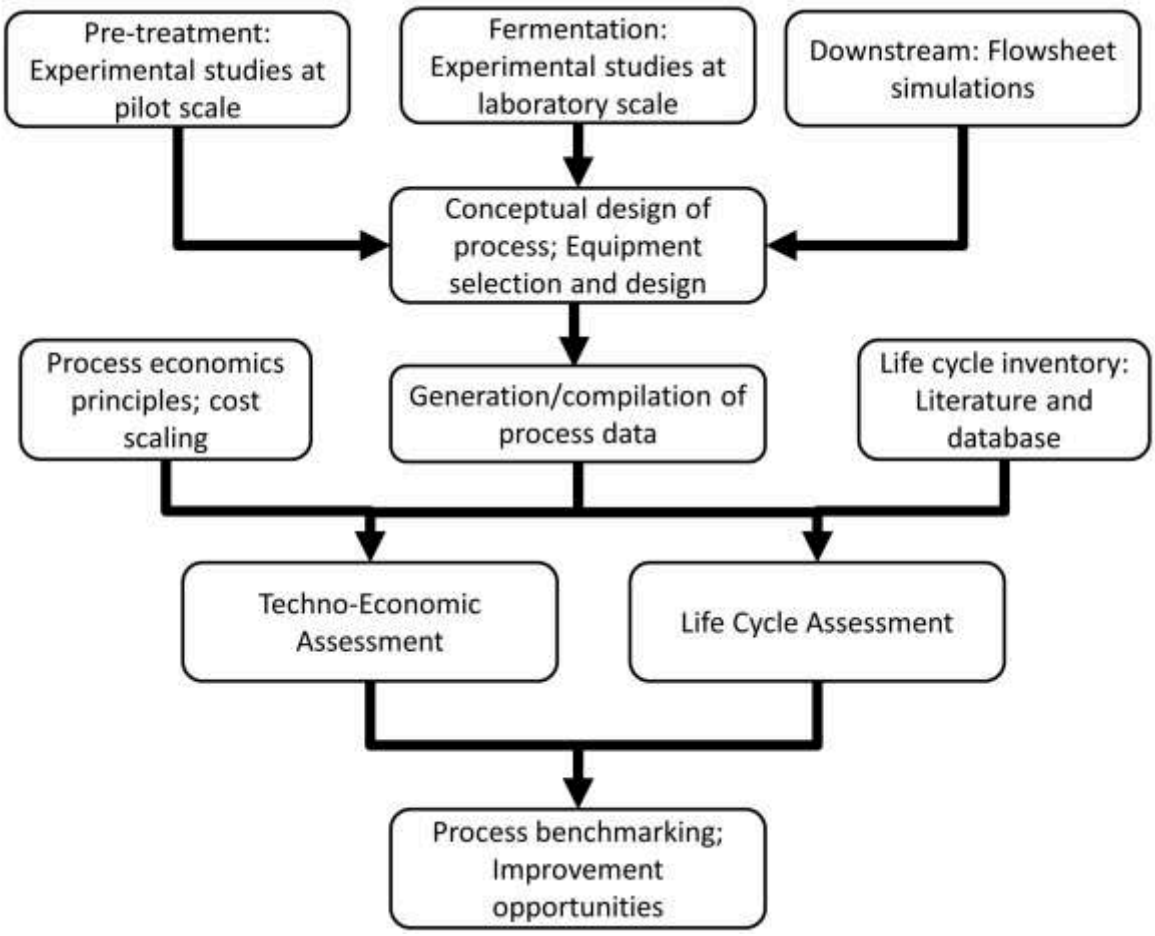
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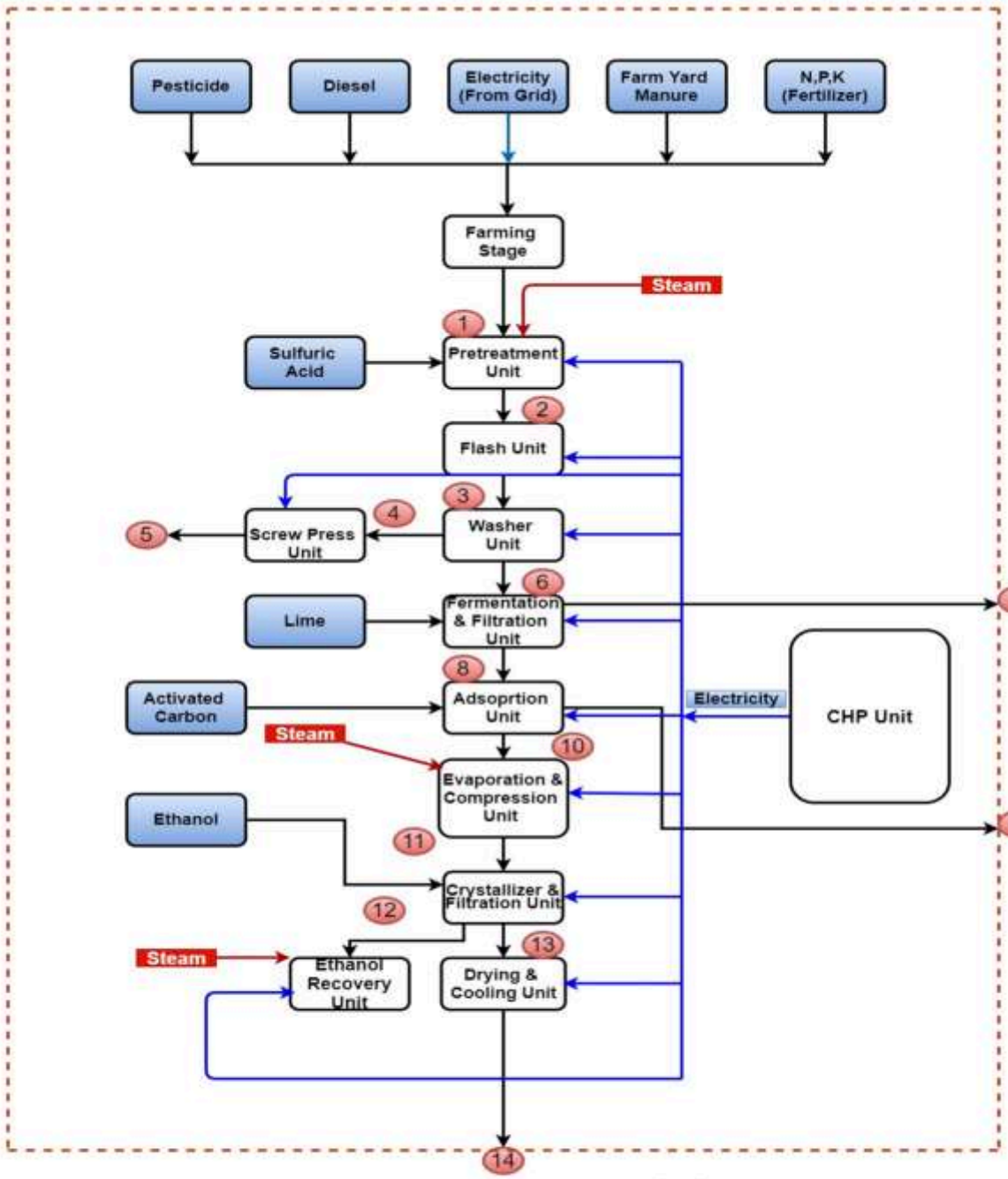
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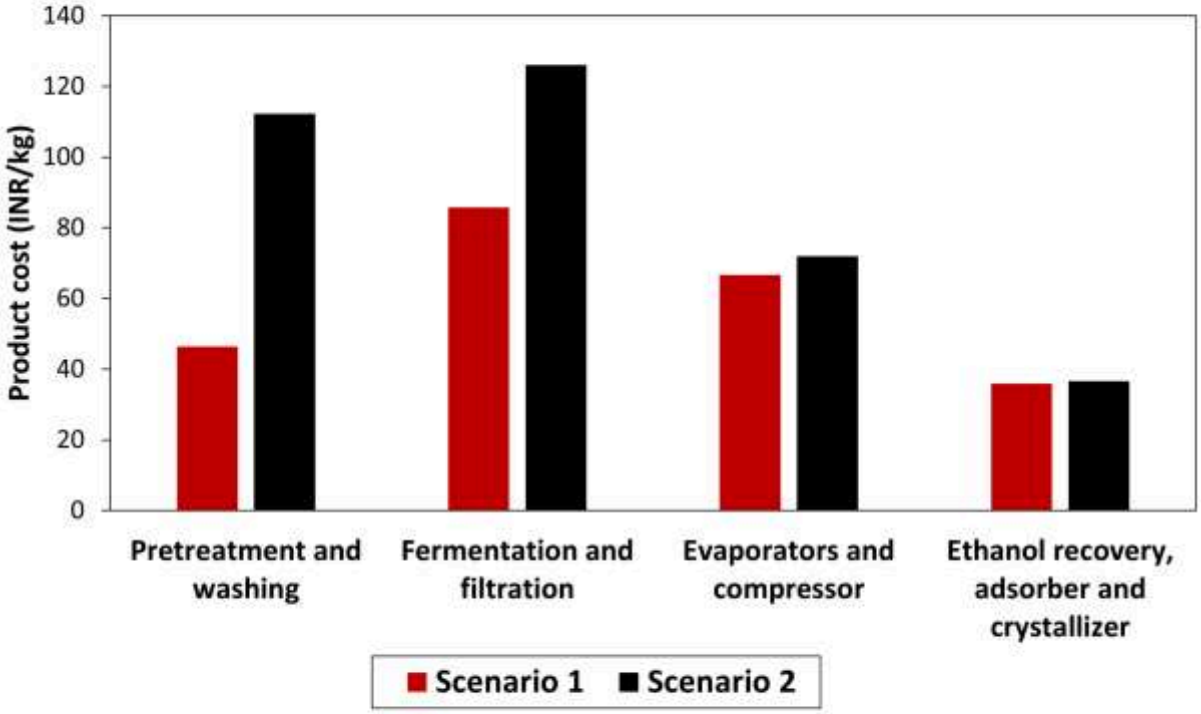
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1: Bagasse
2: Xylose + Water + Sulfuric Acid +Cellulignin + Condensate
3 : Condensate
4 : Xylose + Water + Sulfuric Acid + Cellulignin + Condensate
5 : Xylose + Water + Cellulignin
6 : Xylose + Water + sulfuric acid
7 : Lime + Calcium Sulfate
8 : Xylitol + Water + Impurities
9 : Impurities
10 : Xylitol + Water
11 : Xylitol + Water + Ethanol
12 : Water + Ethanol
13 : Xylitol + Water
14 : Xylitol

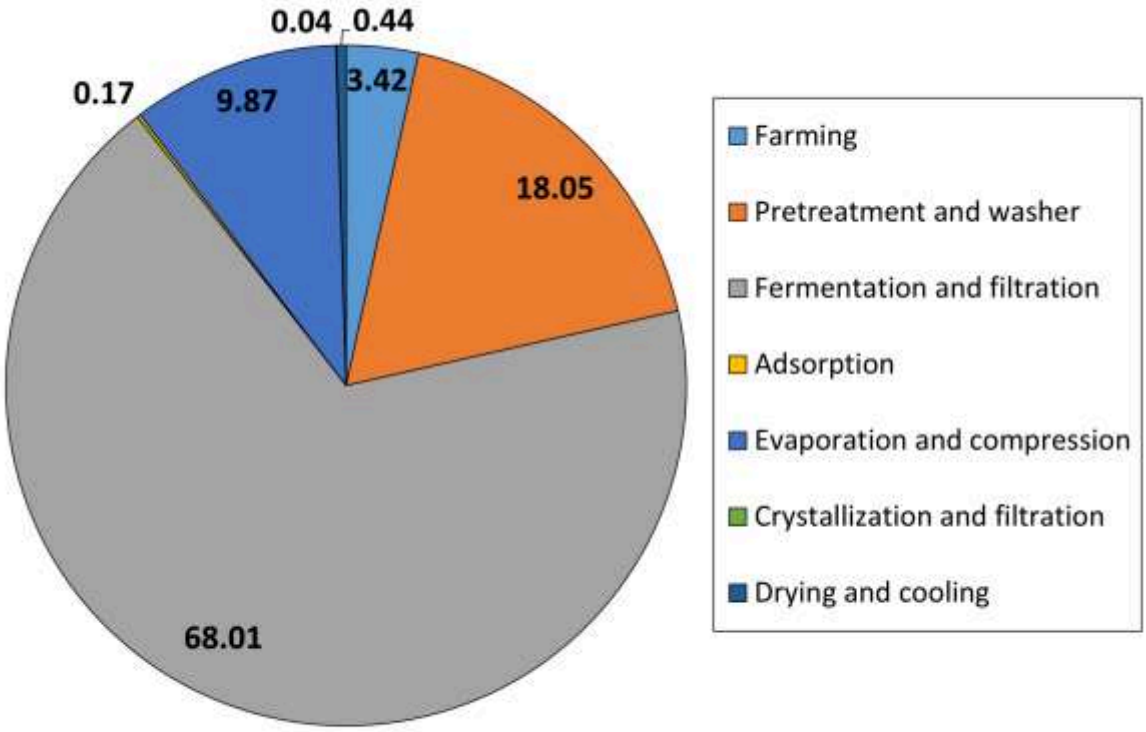
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Sugarcane bagasse valorization to xylitol: techno-economic and life cycle assessment

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