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Economic and Environmental Assessment of Succinic Acid Production from Sugarcane Bagasse

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Abstract

This work presents techno-economic analysis (TEA) and life cycle assessment (LCA) of a novel bio-refinery producing succinic acid (SA) from sugarcane bagasse. The process consists of acid pretreatment, fermentation, followed by downstream separation and purification. Experimental data for pretreatment and fermentation is adapted for a plant processing 4 t/h of dry bagasse, producing 405 kg/h of succinic acid with the same quantity of acetic acid as side product. Downstream separation is simulated in ASPEN PLUS®. The facility is assumed to be annexed to and heat integrated with an existing sugar mill in India. LCA is performed considering cradle-to-gate scope with 1 kg of SA as the functional unit. The TEA results show that although the process is currently not economically feasible, expected improvements in fermentation yields will make it cost competitive. For expected yield, the product cost of SA is INR 121 /kg ($ 1.61/kg), and the selling price of succinic acid should be INR 178 /kg ($ 2.37/kg) for a pay-back period of 4 years. Pretreatment and fermentation are the biggest contributors to the product cost. The life cycle greenhouse gas (GHG) emissions are 1.39 kg CO_2 eq. per kg succinic acid with electricity as the major contributor. Process improvement opportunities are identified to reduce the costs as well as life cycle impacts.

Keywords: succinic acid; bagasse; xylose; product cost; GHG emissions

Introduction

Succinic acid (SA) is an important bulk chemical with several applications and is listed in the top 12 bulk chemicals by the US Department of Energy (DOE).[1,2] Most of the global succinic acid production currently is using the fossil fuel route with maleic anhydride as the feedstock.[3] Sustainability concerns though have generated interest in the production of succinic acid using bio-based route, particularly using lignocellulosic biomass as the feedstock. Additionally, the management of agricultural waste, which is majorly lignocellulosic in nature, is another relevant problem in some countries. India, being the second largest producer of sugarcane, generates large quantities of sugarcane bagasse waste at the sugar mills. Presently, bagasse is not appropriately handled, and mostly used for heat and power generation.[4] This though is not a desirable use of the bioresource considering the principles of green chemistry and engineering.[5] Inappropriate management of bagasse also leads to loss of potential revenue for sugar mills to hedge against volatility in the sugar markets. These factors point towards greater utilization of bagasse in India for production of chemicals, succinic acid being one option.

The level of bio-based production of SA, however, is low. In 2009, only 5% of the total SA was produced using bio-based feedstocks[6] and the growth has been slow due to the relatively high cost of the bio-based route.[7,8] New bio-based processes are being continuously proposed. However, the processes need to be rigorously assessed, including the role of downstream separation and purification. Systematic techno-economic assessment (TEA) for a commercial scale plant that incorporates heat integration strategies needs to be performed. Additionally, the sustainability of the processes needs to be quantified, because bio-based process, even though based on renewable feedstock, may have greater impacts than conventional fossil-based routes.[9,10]

Klein et al.[11] performed economic assessment of first-generation ethanol production using lignocellulosic biomass with co-production of succinic acid and electricity. A similar study for a sugarcane mill co-producing succinic acid, polyhydroxybutyrate (PHB), and electricity has been reported.[12] The yield of SA during fermentation was identified as the key factor. Co-production of bio-diesel and succinic acid has also been analyzed by Vlysidis et al.[13], and it was concluded that co-production of succinic acid had a significant effect on the overall profitability of the bio-refinery. A study based on succinic acid production using sucrose concluded that capital costs has significant effect on the plant profitability.[14] Stylianou et al.[15] had studied production of SA from municipal solid waste and had performed economic assessment for both batch and continuous fermentation. Life cycle assessment (LCA) has been commonly used to quantify environmental impacts of SA production from bio-based routes.[16-18] An important observation in all of these studies was that electricity was a major contributor to the GHG emissions.

Recently, a new processing route has been proposed that focuses on utilizing five carbon sugars in sugarcane bagasse for the production of succinic acid. The process consists of dilute acid pretreatment developed by Nova Pangaea Technology (UK) followed by separation of xylose from the residue consisting mostly of lignin and cellulose. The xylose is fermented to produce succinic acid, while getting acetic acid as the side product. Laboratory scale studies have shown excellent yields and potential for successful scale-up.[19] The novelty of the proposed process is that it has utilized pentose sugar (xylose) for SA production by *Yarrowia lipolytica*. The yeast is well-known producer of SA and has accumulated SA mostly on glycerol.[20] There are some reports on glucose-based SA production but there is hardly any report on SA production from xylose by *Y. lipolytica* as yeast naturally cannot metabolize xylose, the second most abundant sugar after glucose.[21] Therefore, xylose pathway was introduced into *Y. lipolytica* to enable SA production from xylose.[19] Moreover, it connects an independently developed pretreatment process with fermentation and downstream separation process. The goal of this work is to perform detailed economic and life cycle assessment (LCA) for the proposed process considering commercial scale production in India. The experimental data reported for the upstream steps are combined with flowsheet simulation, and the detailed analysis is completed. The study is expected to quantify the performance of the proposed process, identify specific process improvement opportunities, and assess trade-offs between economic and environmental objectives, if any.

The article is organized as follows. The next section explains the process. After that, the methodology for TEA and LCA is described, including flowsheet simulation and life cycle inventory calculations. Subsequently, the results are reported and discussed, followed by conclusions in the final section.

Process Description

The process has been divided into upstream (Fig. 1) and downstream (Fig. 2) sections. After size reduction, bagasse with 35% moisture content undergoes dilute acid pretreatment at 170 °C for 15 minutes with steam at 11 bar pressure.[22] 60 l of 98% sulfuric acid is added to achieve the desired conditions. For the given quantity of reaction mixture (Table S1 in Supplementary information), this translates to about 5% sulfuric acid (w/w). Water and acid are added separately, and electricity is needed for agitation. Pretreatment leads to depolymerization of xylan present in hemicellulose to xylose, while keeping most of the cellulose and lignin intact. The output from pretreatment at high pressure is sent to a flash vessel for recovering waste water containing organic acids and other minor impurities. The other stream containing xylose and residue is sent to washer and screw press units, which separate xylose in liquid form from the solid residue containing cellulose and lignin. Electricity is the major input here, and the liquid stream containing xylose can be sent through an evaporator or membrane separator, depending on the requirements for the fermentation reactor. In the fermentation reactor, xylose is converted to succinic acid (SA) and acetic acid (AA) using *Yarrowia lipolytica PSA02004*. The fermenter is maintained at 37 °C and 7.5 pH, and the residence time is 72 hours. Sulfuric acid carried over from the pretreatment stage reduces the pH, and hence $Ca(OH)_2$ (calcium hydroxide) is added for maintaining the desired pH. This leads to the formation of $CaSO_4$ as a byproduct. The output from the fermenter is fed to a filtration unit that filters $CaSO_4$, and the liquid stream containing succinic acid, acetic acid, and unreacted xylose is the feed to the downstream section for separation and purification.

The feed to the downstream section has 6.66% of SA and AA each, 86.08% of water, and 0.71% of xylose (by weight). In the downstream section, the liquid stream is first preheated to 100 °C and then fed to a reactive distillation column with ethanol as the solvent. In reactive distillation, succinic acid and acetic acid convert to diethyl succinate and ethyl acetate, respectively, and water is formed in this process. The reaction is catalyzed by the Amberlyst 70 and the reaction is second order pseudo-homogeneous.[23] The diethyl succinate and ethyl acetate are obtained at the bottom and top of the column, respectively. Diethyl succinate is sent to a hydrolysis unit, in which it is hydrolyzed to form succinic acid and ethanol. Ethyl acetate is sent to another hydrolysis unit, in which it is hydrolyzed to form acetic acid and ethanol. The distillation column is operated such that 99.8% pure acetic acid is obtained. The succinic acid is sent to an evaporative crystallizer, which evaporates water, and the product stream from the crystallizer containing succinic acid and xylose is obtained.[24] The xylose is filtered as the supernatant, and finally, 99.9% pure succinic acid is recovered. In addition to this main flowsheet, the process also includes ethanol recovery section for ethanol recycle, which is from in both hydrolysis units. Steam required in the process is generated in a boiler which uses solid residue from the pretreatment reactor as the fuel.

Process scale-up and flowsheet development

Based on the process described in the previous section, a flow sheet for a commercial scale plant treating 4 dry tonnes/h plant is developed. This throughput was selected since pretreatment experiments have been conducted for this throughput, and consequently, accurate plant performance as well as equipment cost data are available. The composition of cellulose, hemicellulose and lignin varies with cultivating variety as well as from batch to batch. The broad composition of these three polymeric materials in sugarcane bagasse is as follows: cellulose (42-51%), hemicellulose (18-26%), lignin (17-23%).[25,26] This study assumes hemicellulose percentage to be 25%. Prabhu et al.[19] reported SA yield of 0.15-0.20 g per g of xylose, which can be further improved. Literature has also reported yields in the range of 0.43-0.79 g per g of xylose.[27,28] Therefore, the yield of both succinic and acetic acid is taken as 0.5 g per g xylose. The corresponding concentration and productivity of SA were 66.7 g/l and 0.92 g/l.h, respectively. This results in the annual production of 3,206.8 tonnes of SA. Given the importance of concentration and yield on the process sustainability, calculations are also performed for the values obtained in experimental studies. Table S1 in Supplementary Information provides the process data for the assumed yield and concentration values. The data for the upstream section are based on experimental studies. The downstream process after fermentation is modeled using ASPEN Plus® to obtain the material and energy balances as well as equipment sizes. The NRTL (Non-Random Two Liquid) thermodynamic model is used in ASPEN Plus®. All the distillation columns are modeled using the RADFRAC unit. The esterification of succinic acid and acetic acid is modeled using a reactive distillation column. The column has 12 stages, and stage 3 to 9 are reactive (esterification) stages.[23] The hydrolysis units, are again reactive distillation columns. However, they are modeled as a reactor (RSTOICH reactor model) followed by a distillation column due to lack of reaction kinetics data. Presence of excess water causes the reaction to go to completion by use of a suitable cation exchange resin.[29,30] Finally, the crystallizer is modeled as an evaporative crystallizer using the crystallizer block in ASPEN Plus®.

It is assumed that steam and electricity would be provided by the sugarcane mill, which already houses a combined heat and power (CHP) unit. Additionally, the sugarcane facility also has a cooling tower, which would be used for cooling water recycle from the succinic acid plant. Heat integration is performed to reduce the utility cost requirement. The steam from the boiler is at saturation temperature and pressure of 145°C and 4.14 bar(g) for the downstream section. Moreover, for the pretreatment reactor, the steam is at a pressure of 10 bar(g). The steam after feeding to all the downstream units and pretreatment reactors is returned to the boiler with an assumption of 5% addition of fresh boiler feed water (make-up). Cooling water is also required for the condensers and the heat exchangers in the downstream section. Using the ASPEN Plus® utility option, the mass flow rate of the cooling water is calculated. The cooling water is fed back to the cooling tower with an assumption of a 6% loss in the cooling tower (combination of evaporative loss and blowdown). The calorific value of the solid residue obtained from the pretreatment reactor is assumed to be 14.08 MJ/kg, which is lower than that of bagasse (19.6 MJ/kg). The total steam generated in the boiler in order to meet the steam requirement for the downstream unit is 32,260 kg/h.

TEA and LCA methodology

This section describes the methodology adopted for the TEA and LCA calculations.

TEA methodology

The TEA calculations are based on the methodology proposed by Sinnot and Towler.[31] The equipment cost for upstream section including pretreatment, flash vessel, washer, and screw press is provided by Nova Pangaea Technology (UK). Since the residence time in fermenters is 72 hours, three fermenters will be needed to ensure continuous downstream operations. The volume of each fermenter is 152.8 m^3, and is calculated based on the volumetric flow rate of the liquid feed with additional 10% of head space volume. The costs of fermenters are based on those reported by Davis et al.[32]**,** adjusting for the capacity as well as year. The fermenters require the provision for the aeration, which can be provided by using the compressor pump. The equipment cost of the downstream section is adopted from ASPEN Plus® economic analyzer. The currency conversion factors of 85 and 70 are used for Euros and US Dollars (USD), respectively, to convert equipment costs Indian Rupees (INR). The equipment costs are further reduced by 30% to account for lower labor cost of fabrication in India. All the equipment costs are adjusted for year 2019 using the chemical engineering plant cost index (CEPCI). The equipment costs for heat exchangers and filtration units are taken from the www.Matche.com. The capital costs for cooling tower and the CHP unit are not considered based on the assumption that an existing sugar mill has all these facilities. The procurement cost is considered to be 15% more than the purchase cost of equipment. Further, the fixed capital investment (FCI) is calculated by assuming that procurement cost is 40% of the FCI. Working capital is considered to be 15% of the FCI, and the FCI and working capital give the total capital investment (TCI). These factors are based on feedback provided by engineering design companies in the Indian context.

The raw material costs are taken from the www.indiamart.com except for the catalyst. The catalyst loading for the two hydrolysis units is 76 kg/m^3 based on the values reported in literature.[23] The cost of catalyst is adapted from Guan et al.[33] The raw material costs are show in Table S2 in Supplementary Information. The utilities include process water, boiler feed water, cooling water, and electricity. All the electricity requirements and steam requirements are met by using the CHP unit. The cost of electricity is assumed to be 6 INR/kWh. The boiler feed water cost is 90 INR/m^3 , while the process water and cooling water costs are 20 INR/m^3.[34] A recycle rate of 10%, 5%, and 6% for process, boiler feed, and cooling water, respectively, is assumed. For the fermentation tanks, the aeration rate for the fermenter is 2 liters per minute for 1 liter of fermentation liquid, and this determines the electricity required by compressors. The total economic life of the plant is 10 years and with 330 working days per year.

In TEA, two scenarios have been compared. In scenario 1, bagasse and electricity are considered to be free, available from the sugar mill. In contrast, scenario 2 assumes that they need to be purchased. Additionally, sensitivity analysis is done to understand the dependence of succinic acid yield on the costs. For each case, the product cost of SA has been calculated. This is the per unit cost of SA production considering the operating and capital expenses. It provides the absolute lower bound on the selling price and does not directly provide information regarding profitability. For that, detailed cash-flow calculations are performed considering the annual expenses, revenues, profit as well as taxes. A tax rate of 30% in income is considered. Payback period is the time in which capital investment is recovered, and a payback period of four to six years is desirable. Therefore, the selling price of SA at which payback period of four years is achieved has been determined by trial and error and has been reported. The selling price of acetic acid is fixed at Rs. 70 /kg ($ 1 /kg) for this calculation.

LCA methodology

The goal of this study is to quantify the life cycle impacts of SA production, which can be used by process developers for further reducing the impacts. Similarly, the study can be used to assess the benefit of producing bio-based SA as compared to fossil-based SA. The scope for LCA study is cradle-to-gate and includes the farming, transportation, and the processing stages (Fig. 3). 1 kg of succinic acid is taken as the functional unit. Table S1 in Supplementary Information reports the reference flows. The life cycle inventory data for inputs such as electricity, lime, and sulfuric acid are taken from the Ecoinvent® database (version

3.3). Data for India are used if available, such as for electricity. Otherwise, inventory data for RoW (Rest of the World) are used. The LCA model is developed using the OpenLCA software version 1.10.2, and Recipe (H) Midpoint method is used for impact assessment. Economic allocation is performed to divide the total impacts into succinic and acetic acid.

Results and discussions

This section first summarizes the TEA results and then discusses the LCA results.

Techno-economic assessment results

Table 1 summarize the key TEA results for the two scenarios and Fig. 4 shows the break-up of the total product cost among the various stage of the process. For scenario 1, the product cost of succinic acid is INR 121.5 /kg ($ 1.73 /kg), and selling price of INR 178 /kg ($ 2.54 /kg) leads to a pay-back period of four years. The pretreatment section, which includes the pretreatment reactor, flash unit, washer, and screw press unit, contributes 44% of the total product cost, followed by the fermentation unit and compressors (28%). In the downstream section, the hydrolysis unit contributes significantly to the total production cost of the plant. The product cost is dominated by capital cost component, and 71 % of the total equipment cost is due to the pretreatment reactor and its ancillary units. This is due to the expensive material of construction to handle high pressure conditions and presence of dilute H_2SO_4. The recycling of solvent (ethanol), process, cooling, and finally the boiler feed water (condensate) significantly reduce the operating cost. If the economic life of the plant is assumed to be 15 and 20 years (instead of 10 years as considered previously), the product cost is INR 96.68 /kg ($ 1.38 /kg) and INR 104.9 /kg ($ 1.49 /kg), respectively. Instead, if the desired payback period is changed seven years with 10 years economic life of the plant, the selling price reduces to INR 120 /kg ($ 1.71 /kg). For intermediate pay back periods, the selling price will be within this range. 25% reduction in the pretreatment equipment cost reduces the product cost to INR 111 /kg ($ 1.58 /kg), and the selling price can be INR 150 /kg ($ 2.14 /kg) for a payback period of 4 years. The corresponding product cost and selling price numbers for 50% reduction in capital cost of upstream section are INR 100 /kg ($ 1.42 /kg) and INR 130 /kg ($ 1.86 /kg), respectively.

For scenario 2, the economic outlook is less optimistic due to the additional costs of bagasse and electricity. The product cost of succinic acid is INR 252.7 /kg ($ 3.61 /kg), and the selling price needs to be INR 300 /kg ($ 4.28 /kg) to achieve a payback period of four years. This is an increase of 68% as compared to scenario 1. Compared to scenario 1, the share of raw material and utility cost increases significantly, since the upstream section is highly energy-intensive. The total electricity requirement in the plant is 1727 kW, out of which 72.5% is required for the fermentation unit and 27 % is required in the pretreatment section. This is also reflected in the stage-wise break-up of the total product cost (Fig. 4). The solid residue from the pretreatment reactor can only meet 50% of the total steam requirement, and bagasse, in addition to being the process input, is also required for steam generation. Thus, the total bagasse loading for the entire plant is 6,420 kg/h, out of which 2,420 kg/h is required for the steam generation.

The results of this work are consistent with the reported market price of $ 3-8 /kg for succinic acid from the petroleum route.[8] However, this study makes some assumptions such as validity of laboratory scale results for a commercial plant. Moreover, issues such as feedstock composition variability as well as raw material and utility cost fluctuations are ignored. Therefore, the results should be considered as optimistic estimates. When compared with analysis of other bio-based processes, the results are promising. Klein et al.[11] determined the selling price of succinic acid to be 2.32 $/kg, while Nieder-Heitmann et al.[12] reported selling price of between 1.5-2.5 $/kg for various scenarios. Co-production of succinic acid and co-generation of electricity in a sugarcane mill has been found to greatly increase the economic feasibility in all these cases. Stylianou et al.[15] determined the minimum selling price of SA produced from municipal solid waste to be $ 2.5/kg when continuous fermenters were used with a capacity of 40,000 t/y of SA.

Life cycle assessment results

Table 2 reports life cycle impacts for selected impact categories, and detailed results are reported in Table S4 in Supplementary Information. All values are for 1 kg of SA. The climate change impact is 1.39 kg CO_2

eq., and the contribution of various stages of the process is shown in Fig. 5. The biggest contributor to climate change impact is the fermentation unit (60.06%) due to electricity required in aeration. Although the electricity is produced from bagasse, it still has some impact due to farming stage as well as the actual electricity production stage. The upstream part utilizes a significant amount of electricity for its applications. Additionally, lime is added to neutralize the H_2SO_4, which contributes to the CO_2 emission. In the downstream section, the usage of raw materials such as ethanol also add to the overall climate change impact. The climate change impacts are significantly reduced due to the usage of CHP unit to generate electricity, which has a GHG emission factor of 0.28 kg CO_2 eq. per kWh. For electricity grid mix in India, the GHG emission factor is 1.23 kg CO_2 eq. per kWh. If this electricity is considered, the total climate change impact will be 4.30 kg CO_2 eq per kg of SA.

The life cycle water depletion is 2.15 m^3 per kg of SA. The water depletion is highest in the fermentation unit due to the electricity requirement and the addition of lime. Electricity production (using CHP) contributes to the 1.42 m^3 water per kWh (Ecoinvent 3.3 database). Human toxicity majorly arises from the release of metals such as arsenic, lead, and selenium during the combustion of fuels during the various production process. The electricity usage in the upstream part contributes to the majority of total human toxicity emissions. The particulate emissions are high due to the usage of bagasse in the boiler. The emissions for particulate matter is 0.005 kg PM_{10} per kg succinic acid. However, the PM emissions can be controlled using a device such as a wet scrubber and bag filters.

The climate change impact for 1 kg of succinic acid from fossil-based route has been reported to be 1.9 kg CO_2 eq.,[16] which is 36.7% higher than that for the process considered here. Smidt et al.[16] reported the life cycle GHG (greenhouse gas) emission for SA production from dextrose obtained from corn to be 0.85 kg of CO_2 eq. per kg SA. Moussa et al.[17] reported the climate change impact of 0.87 kg CO_2 eq. per kg succinic acid obtained from glucose. The study is done based on the Myriant bio-refinery Louisiana, USA. However, in this study, the impacts are also allocated to ammonium sulfate, which is an important co-product in the process. Morales et al.[35] studied bio-based succinic acid production routes from sugar beet and wood residue, and also identified the significant contribution of fermentation section to the total CO_2 emissions. Cok et al.[18] reported the climate change impact values to be between 0.88-1.47 kg CO_2 per kg succinic acid from corn starch using different downstream processing routes. These comparisons indicate that the current process is comparable to those discussed in literature. It also indicates that with cleaner electricity options, the impact can be further reduced.

Impact of succinic acid yield

The yield and concentration of succinic acid in the fermentation broth will have a significant impact on the techno-economic feasibility as well as life cycle assessment results presented before. The TEA and LCA results are determined for the experimentally obtained yield of 0.14 g/g. Results show that for scenario 1, the product cost increases to INR 410 /kg ($ 5.85/kg), which is almost 3.4 times that for the value reported previously. This is expected since lower yield reduces the total SA produced from the same quantity of bagasse. This results in reduced revenue and lower return on capital investment. The selling price to obtain a payback period of four years in this case is INR 720 /kg ($ 10.3/kg). Lower yield also affects the life cycle impacts. The life cycle climate change impact is 4.91 kg of CO2 eq./kg of SA, which is 3.53 times higher than the impact reported previously.

As mentioned previously, it is expected that a higher yield of 0.5 g/g can be achieved. However, the impact of change in the SA yield around this targeted yield on the economic feasibility is also determined by varying the SA yield to 0.4 and 0.6 g/g of xylose around the base case value of 0.5 g/g of xylose for the same bagasse throughput. The corresponding concentrations of succinic acid are 53.36 g/l and 80.04 g/l. The results (Fig. S2 in Supplementary Information) show an almost linear variation of product cost with respect to the yield of succinic acid. The product costs for SA yield of 0.4 g/g xylose and 0.6 g/g xylose are INR 149 /kg ($ 2.12 /kg) and INR 102 /kg ($ 1.46 /kg), respectively. The variation is due to less or more efficient use of capital investment in the downstream section. Increase in yield increases the load on the crystallizer unit. However, this increase in equipment cost is compensated by greater revenue from SA. Table S6 in Supplementary Information provides detailed breakdown of the cost and the selling price desirable for four years payback period.

Conclusion

This work performed a detailed techno-economic and life cycle assessment of a novel process to utilize xylose obtained from sugarcane bagasse to produce succinic acid. A combination of experimental data and process flowsheet simulation were used to generate the necessary data. The techno-economic analysis results showed that the process feasibility strongly depended on the yield of succinic acid during the fermentation stage. Although the process is not economically feasible for the yield achieved currently in the laboratory, higher yields are achievable, and for such yields, the proposed process can be cost-competitive with the existing fossil-based route. Pretreatment and fermentation were identified as the major cost components, and therefore further cost reduction opportunities must be explored for these steps. The availability of bagasse and electricity at no cost from sugar mill made a significant reduction in the total product cost. However, the results reported here were optimistic estimates as they ignored some of the practical challenges such as feedstock supply fluctuations. The life cycle assessment results showed that while the climate change impacts were lower than those for the fossil-based route, the difference was not significant. This meant that greater improvement is required to achieve significant environmental benefits. These improvements could be in terms of improved yields in the fermentation stage or reduced energy requirement in the pretreatment and separation stage. Electricity production is the major contributor to the overall emissions due to high electricity requirement in the upstream section. The overall emissions were significantly reduced due to the utilization of bagasse from the sugar mill to produce electricity. The work can be extended to consider additional processing options to set-up an integrated biorefinery. The solid residue obtained after pretreatment is rich in cellulose and lignin and is being explored as feedstock for anaerobic digestion to produce bioCNG.

Supporting Information

Detailed process data tables, raw material costs, LCA process inventory, LCA impacts table, ASPEN Plus flowsheet and stream data, impact of yield variation on economics

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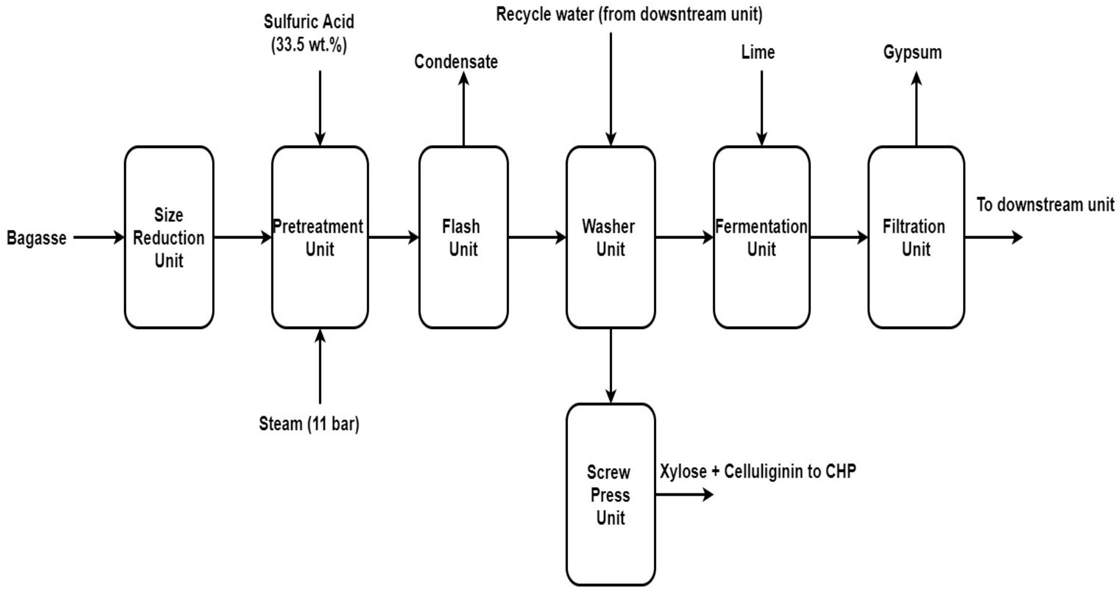

Figure 1: Upstream section (pretreatment and fermentation) of succinic acid production from sugarcane bagasse

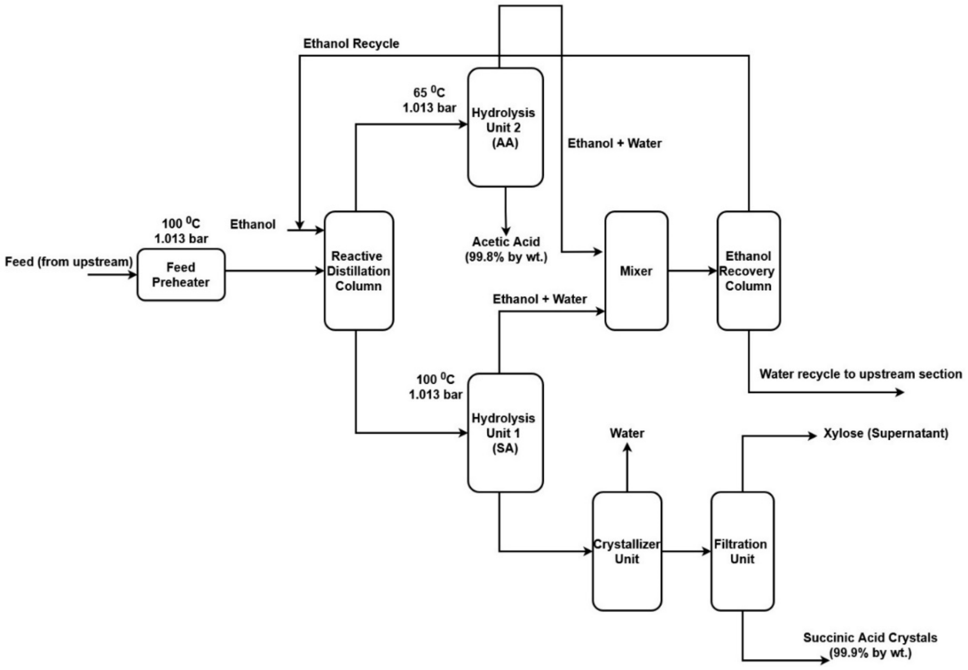

Figure 2: Downstream section of succinic acid separation and purification

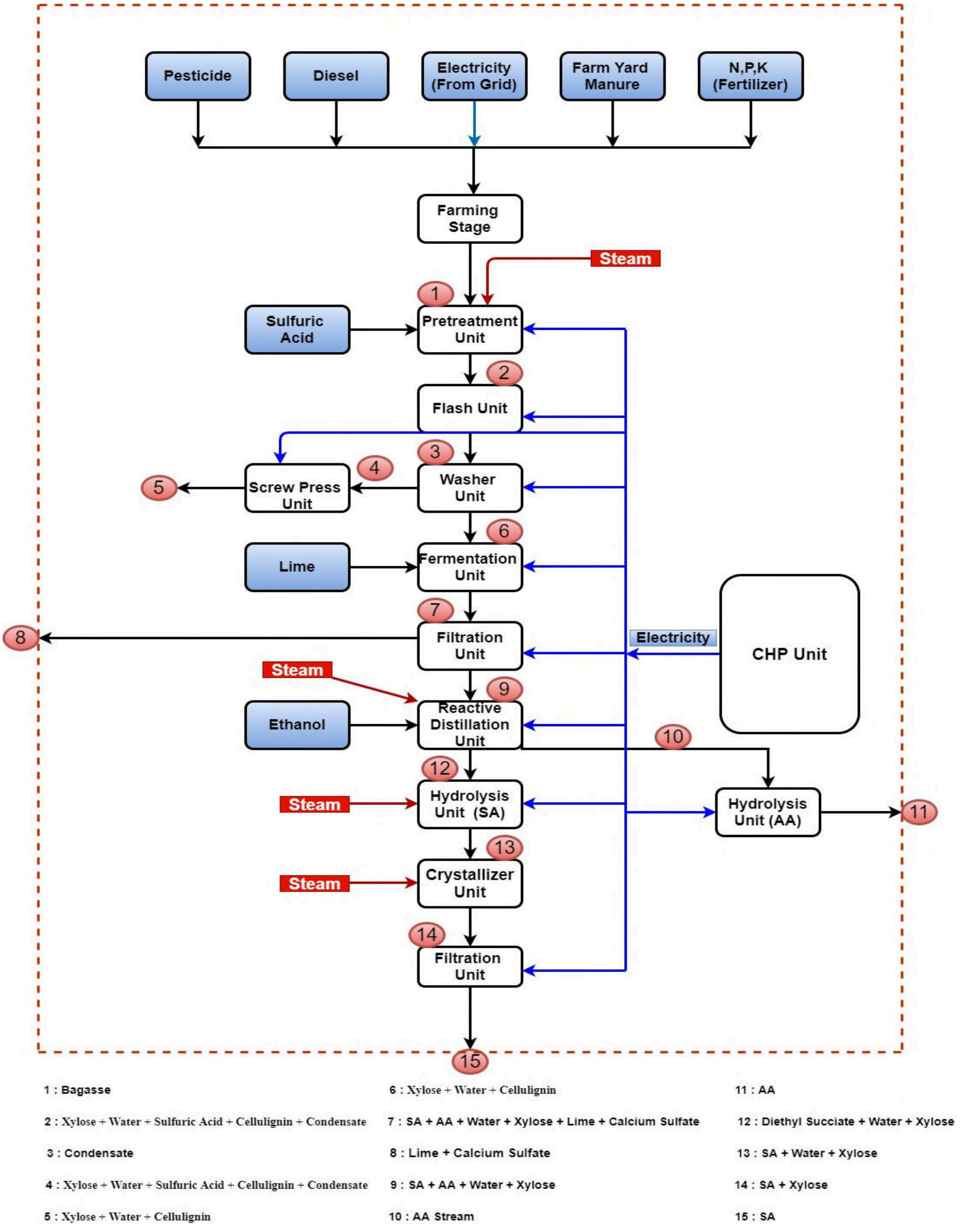

Figure 3: System boundary and product system LCA of succinic acid production from sugarcane bagasse

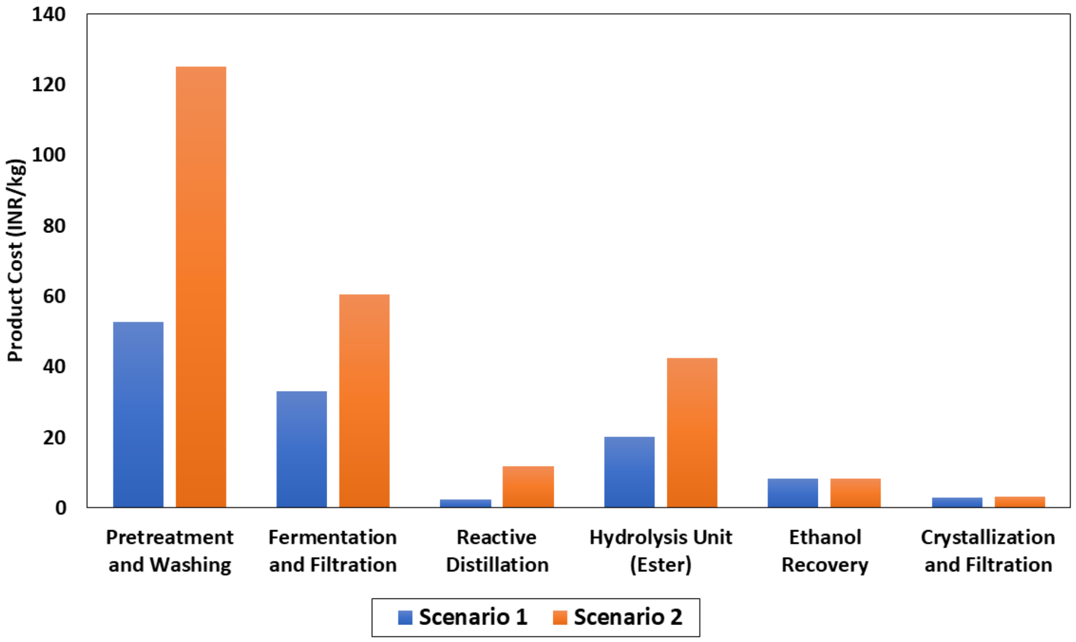

Figure 4: Distribution of succinic acid product cost among the various process stages for two scenarios. Scenario 1 considers electricity and bagasse available for free, while Scenario 2 considers they are not free.

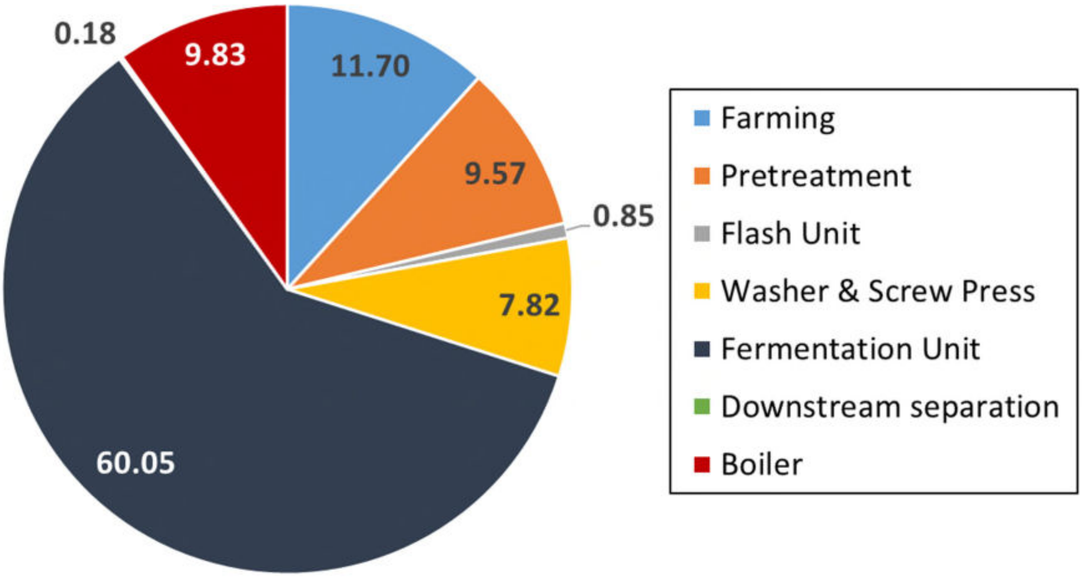

Figure 5: Distribution of the total climate change impact for the production of 1 kg of succinic acid among the various stages of the process

Table 1: Results of techno-economy assessment of succinic acid production from sugarcane bagasse for both scenarios

Parameter	**Scenario 1**	**Scenario 2**
Product cost (INR/kg)	121.45 ($ 1.73 /kg)	252.72 ($ 3.61 /kg)
Selling price for four-year payback period (INR/kg)	178 ($ 2.54 /kg)	300 ($ 4.28 /kg)
Rate of return (ROR)%	19.31	17.89
NPV (INR Million)	941.65 ($ 13.4 Million)	764.66 ($ 10.9 Million)
Raw material cost (INR Million)	11.82 ($ 0.168 Million)	215.20 ($ 3.07 Million)
Utilities cost (INR Million)	9.83 ($ 0.14 Million)	91.89 ($ 1.31 Million)
Purchased equipment cost (INR Million)	442.08 ($ 6.31 Million)	442.08 ($ 6.31 Million)

Table 2: Life cycle impacts for production of 1 kg of succinic acid for selected impact categories

Impact category	**Overall impacts for the process**
Climate Change (kg CO_2 eq)	1.390
Fossil depletion (kg oil eq)	0.209
Freshwater ecotoxicity (kg 1,4-DB eq)	0.012
Freshwater eutrophication (kg P eq)	0.001
Human toxicity (kg 1,4-DB eq)	0.439
Particulate matter formation (kg PM_{10} eq)	0.036
Photochemical oxidant formation (kg NMVOC)	0.026
Water depletion (m^3)	2.150

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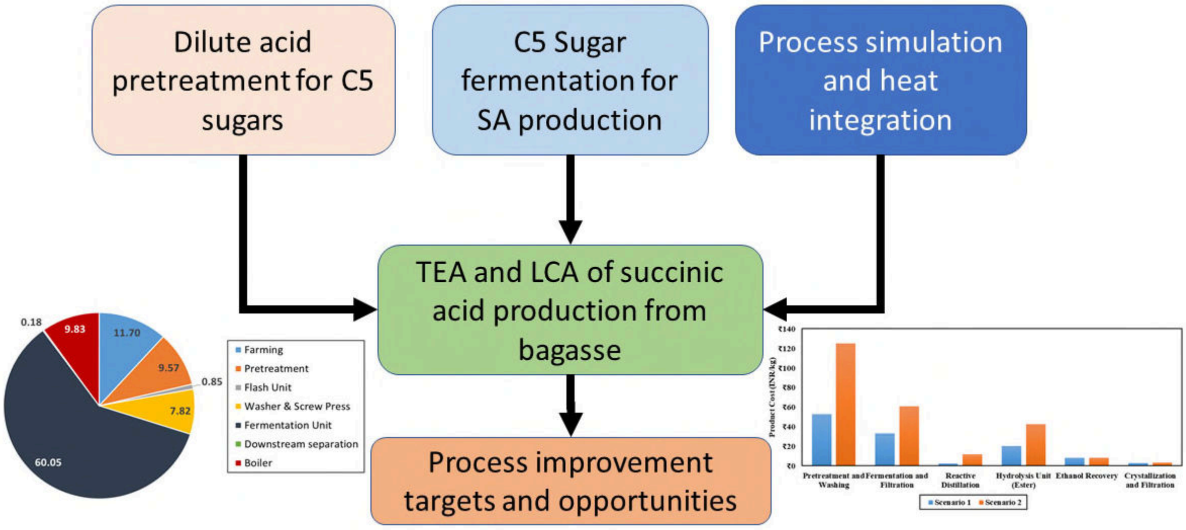

Synopsis: Economic and life cycle assessment of novel succinic acid production process from bagasse shows commercialization potential and climate change benefits.

Supporting Information

Economic and Environmental Assessment of Succinic Acid Production from Sugarcane Bagasse

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Table S1: Detailed process data for the processing of 4 tonnes/h of bagasse

S. No.	Input	Value	Output	Value
1	***Farming stage (bagasse for the process)***			
	Electricity (kW)	**26.32**	Bagasse (kg)	**4000**
	Diesel (kg)	**4.45**		
	Water (kg)	**974594.3**		
	Nitrogen (kg)	**9.72**		
	Phosphorous (kg)	**3.24**		
	Potassium (kg)	**3.24**		
	Farm yard Manure (kg)	**356.72**		
	Pesticides (kg)	**0.32**		
2	***Farming stage (bagasse for the steam production)***			
	Electricity (kW)	**15.7911**	Bagasse (kg) (for steam production)	**2408.5**
	Diesel (kg)	**2.8343**		
	Water (kg)	**589534.4**		
	Nitrogen (kg)	**5.6686**		
	Phosphorous (kg)	**2.0245**		
	Potassium (kg)	**2.0245**		
	Farm yard Manure (kg)	**214.597**		
	Pesticides (kg)	**0.20245**		
3	***Boiler Unit***			
	Bagasse (kg)	**2408.5**	Steam (kg)	**34260**

	Water (kg)	**34260**		
4	***Pretreatment Reactor***			
	Bagasse (kg)	**4000**	Product Stream 1 (kg)	**8332.84**
	Electricity (kW)	**235**		
	Water (kg)	**133.21**		
	Steam (kg)	**2000**		
	Sulfuric Acid (l)	**60**		
5	***Flash Unit***			
	Electricity (kW)	**22.80**	Product Stream 2 (kg)	**7810.12**
	Product Stream 1 (kg)	**8332.84**	Condensate (kg)	**523.13**
6	***Washer Unit***			
	Electricity (kW)	**150**	Product Stream 3 (kg)	**6067.02**
	Water (kg)	**3905**	Product Stream 4 (kg)	**7839.67**
	Product Stream 2 (kg)	**7810.12**		
7	***Screw Press Unit***			
	Electricity (kW)	**61**	Xylose (kg)	**90**
	Product Stream 4 (kg)	**7839.67**	Cellulignin (residue) (kg)	**3100**
8	***Fermentation Unit***			
	Electricity (kW)	**1251.95**	Product Stream 5 (kg)	**6283.64**
	Lime (kg)	**112.56**		
	Product Stream 3 (kg)	**6067.02**		
9	***Filtration***			
	Product Stream 5 (kg)	**6283.64**	Product Stream 6 (kg)	**6132.62**
	Electricity (kW)	**1**	Gypsum (kg)	**83.41**

10	***Feed Preheater & Reactive Distillation Unit***			
	Product Stream 6 (kg)	**6132.62**	Diethyl Succinate Stream (kg)	**3439.63**
	Ethanol + Water (kg)	**675**	Ethyl acetate Stream (kg)	**3346.09**
	Steam (kg)	**5306.46**		
11	***Hydrolysis Unit (AA)***			
	Ethyl acetate Stream (kg)	**3346.09**	AA (kg) (99.8% by wt.)	**401**
	Electricity (kW)	**1**	Ethanol Stream (kg)	**2945**
	Steam (kg)	**13575.27**		
12	***Hydrolysis Unit (SA)***			
	Diethyl Succinate Stream (kg)	**3439.63**	SA Stream (kg)	**661.80**
	Electricity (kW)	**1**	Ethanol Stream (kg)	**2800**
	Steam (kg)	**11297.18**		
13	***Ethanol Recovery Unit***			
	Ethanol Stream (kg)	**5745**	Ethanol + Water (kg)	**675**
	Electricity (kW)	**1**	Water (kg)	**5070**
	Steam (kg)	**1921.40**		
14	***Crystallizer Unit***			
	SA Stream (kg)	**661.80**	Water (kg)	**213.14**
	Steam (kg)	**160.05**	SA + Xylose (kg)	**448.66**
15	***Filtration Unit***			
	SA + Xylose (kg)	**448.66**	Xylose (kg)	**43.36**
	Electricity (kW)	**1**	SA (kg) (99.9% by wt.)	**405.30**

Table S2: Raw material costs used for economic calculations.

S.No.	**Component**	**Cost per kg (INR/kg)**	**Flow Rate (kg/hr)**	**Cost Per Day (INR/day)**	**Cost Per Year (INR/year)**
1	Sulfuric Acid	₹ 13.00	60	18720	₹ 6,177,600
2	Ethanol	₹ 45.00	0.067	72.36	₹ 23,878
3	Catalyst (RD)	₹ 276.00			₹ 364,562
4	Catalyst (SAC)	₹ 276.00			₹ 173,052
5	Catalyst (AA)	₹ 276.00			₹ 163,361
6	Lime	₹ 5.50	112.837	14894.484	₹ 4,915,179
7.	Bagasse	₹ 4.00	6420	₹ 616,320.00	₹ 203,385,600

Table S3: Detailed process inventory for the production of 1 kg of succinic acid

Sno	**Input**	**Value**	**Output**	**Value**
1	***Farming stage*** ***(Bagasse for the process)***			
	Electricity (kWh)	**0.065**	Bagasse (kg)	**9.879**
	Diesel (kg)	**0.011**	Nitrogen Oxides (kg)	**0.004**
	Water (kg)	**2407**	Phosphorous runoff (kg)	**0.001**
	Nitrogen (kg)	**0.024**	NH_3 emissions (kg)	**0.0006**
	Phosphorous (kg)	**0.008**		
	Potassium (kg)	**0.008**		
	Farm yard Manure (kg)	**0.881**		
	Pesticides (kg)	**0.0008**		
2	***Pretreatment Reactor***			
	Bagasse (kg)	**9.879**	Product Stream 1 (kg)	**20.580**
	Electricity (kWh)	**0.5804**		
	Water (kg)	**0.329**		
	Sulfuric Acid (kg)	**0.148**		
3	***Flash Unit***			
	Electricity (kWh)	**0.056**	Product Stream 2 (kg)	**19.289**
	Product Stream 1 (kg)	**20.580**	Condensate (kg)	**1.292**
4	***Washer Unit***			
	Electricity (kWh)	**0.37**	Product Stream 3 (kg)	**14.984**
	Water (kg)	**2.778**	Product Stream 4 (kg)	**19.362**
	Product Stream 2 (kg)	**19.289**		
5	***Screw Press Unit***			

	Electricity (kWh)	**0.15**	Xylose (kg)	**0.222**
	Product Stream 4 (kg)	**19.362**	Cellulignin (kg)	**7.656**
6	***Fermentation Unit***			
	Electricity (kWh)	**3.092**	Product Stream 5 (kg)	**15.519**
	Lime (kg)	**0.278**		
	Product Stream 3 (kg)	**14.984**		
7	***Filtration***			
	Product Stream 5 (kg)	**15.519**	Product Stream 6 (kg)	**15.146**
	Electricity (kWh)	**0.0025**	Gypsum (kg)	**0.206**
8	***Reactive Distillation Unit***			
	Product Stream 6 (kg)	**15.146**	Diethyl Succinate Stream (kg)	**8.495**
	Ethanol (kg)	**0.0002**	Ethyl acetate Stream (kg)	**8.264**
	Electricity (kWh)	**0.0025**		
9	***Hydrolysis Unit (Succinic Acid)***			
	Diethyl Succinate Stream (kg)	**8.495**	Succinic acid stream(kg)	**1.580**
	Electricity (kWh)	**0.0025**	Ethanol Stream(kg)	**6.915**
10	***Crystallization and Filtration Unit***			
	Succinic acid stream(kg)	**1.580**	Succinic acid (kg)	**1.000**
	Electricity (kWh)	**0.0025**		
11	***Farming stage (Bagasse for steam production)***			
	Electricity (kWh)	**0.039**	Bagasse (kg)	**5.948**
	Diesel (kg)	**0.007**	Nitrogen Oxides (kg)	**0.002**

	Water (kg)	**1456**	Phosphorous runoff (kg)	**0.0006**
	Nitrogen (kg)	**0.014**	NH_3 emissions (kg)	**0.0003**
	Phosphorous (kg)	**0.005**		
	Potassium (kg)	**0.005**		
	Farm yard Manure (kg)	**0.53**		
	Pesticides (kg)	**0.0005**		
12	***Boiler***			
	Bagasse (kg)	**5.948**	Steam (kg)	**84.61**
			Particular Matter (kg)	**0.030**
			Nitrogen Oxides (kg)	**0.002**
			Poly-organic Matter (kg)	**0.00002**

Table S4: Life cycle impacts for production of 1 kg of succinic acid

S.No.	**Impact category**	**Reference unit**	**Value**
1	Agricultural land occupation	m^2*a	0.950
2	Climate Change	kg CO_2 eq	1.390
3	Fossil depletion	kg oil eq	0.209
4	Freshwater ecotoxicity	kg 1,4-DB eq	0.012
5	Freshwater eutrophication	kg P eq	0.001
6	Human toxicity	kg 1,4-DB eq	0.439
7	Ionizing radiation	kg U_{235} eq	0.045
8	Marine ecotoxicity	kg 1,4-DB eq	0.008
9	Marine eutrophication	kg N eq	0.004
10	Metal depletion	kg Fe eq	0.043
11	Natural land transformation	m^2	0.010
12	Ozone depletion	kg CFC-11 eq	0.000
13	Particulate matter formation	kg PM_{10} eq	0.036
14	Photochemical oxidant formation	kg NMVOC	0.026
15	Terrestrial acidification	kg SO_2 eq	0.020
16	Terrestrial ecotoxicity	kg 1,4-DB eq	0.029
17	Urban land occupation	m^2*a	0.016
18	Water depletion	m^3	2.150

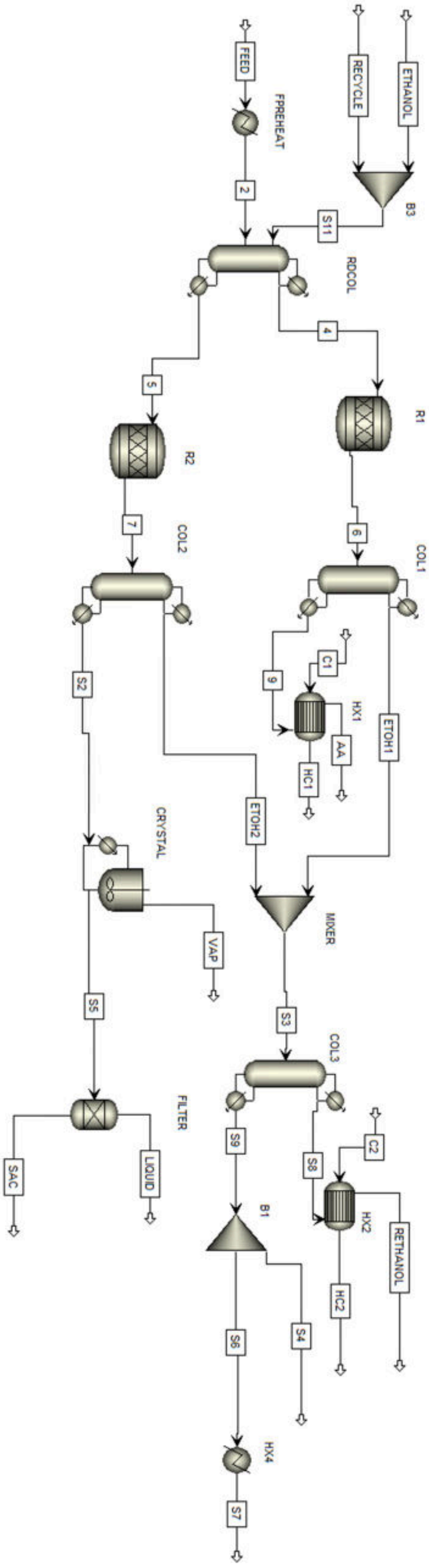

Figure S1: ASPEN Plus flowsheet for downstream separation and purification of succinic acid

Table S5: Stream data for ASPEN Plus flowsheet simulation for each stage. Stream that have zero values are included for the sake of completeness

Feed Preheater					
		Input	**Output**		
Phase		**Liquid**	**Liquid**		
Temperature	**C**	37	100		
Mass Flow	**kg/h**	6132.740	6132.740		
Mass Fraction					
ACETI-01		0.066	0.066		
SUCCI-01		0.066	0.066		
ETHAN-01		0.000	0.000		
WATER		0.861	0.861		
MONOE-01		0.000	0.000		
DIETH-01		0.000	0.000		
ETHYL-01		0.000	0.000		
XYLOS-01		0.007	0.007		
Reactive Distillation Colum					
		Input	**Input**	**Output**	**Output**
Phase		**Liquid**	**Liquid**	**Liquid**	**Liquid**
Temperature	**C**	100.000	30.000	100.629	57.480
Mass Flow	**kg/h**	6132.740	675.058	3461.798	3346.000
Mass Fraction					
ACETI-01		0.066	0.000	0.000	0.001
SUCCI-01		0.066	0.000	0.000	0.000
ETHAN-01		0.000	0.926	0.000	0.000
WATER		0.861	0.074	0.815	0.823
MONOE-01		0.000	0.000	0.000	0.000
DIETH-01		0.000	0.000	0.173	0.000
ETHYL-01		0.000	0.000	0.000	0.176
XYLOS-01		0.007	0.000	0.013	0.000
Reactor 1					
		Input	**Output**		
Phase		**Liquid**	**Liquid**		
Temperature	**C**	57.480	57.478		
Mass Flow	**kg/h**	3346.000	3346.000		
Mass Fraction					
ACETI-01		0.001	0.121		
SUCCI-01		0.000	0.000		
ETHAN-01		0.000	0.092		
WATER		0.823	0.787		
MONOE-01		0.000	0.000		
DIETH-01		0.000	0.000		

ETHYL-01		0.176	0.000		
XYLOS-01		0.000	0.000		
Reactor 2					
		Input	**Output**		
Phase		**Liquid**	**Mixed**		
Temperature	**C**	100.629	100.594		
Mass Flow	**kg/h**	3461.798	3461.798		
Mass Fraction					
ACETI-01		0.000	0.000		
SUCCI-01		0.000	0.117		
ETHAN-01		0.000	0.091		
WATER		0.815	0.779		
MONOE-01		0.000	0.000		
DIETH-01		0.173	0.000		
ETHYL-01		0.000	0.000		
XYLOS-01		0.013	0.013		
Column 1 (AA)					
		Input	**Output**	**Output**	
Phase		**Liquid**	**Liquid**	**Liquid**	
Temperature	**C**	57.478	117.864	91.079	
Mass Flow	**kg/h**	3346.000	401.000	2945.000	
Mass Fraction					
ACETI-01		0.121	0.998	0.002	
SUCCI-01		0.000	0.000	0.000	
ETHAN-01		0.092	0.000	0.105	
WATER		0.787	0.002	0.894	
MONOE-01		0.000	0.000	0.000	
DIETH-01		0.000	0.000	0.000	
ETHYL-01		0.000	0.000	0.000	
XYLOS-01		0.000	0.000	0.000	
HX1 (AA)					
		Input	**Input**	**Output**	**Output**
Phase		**Liquid**	**Liquid**	**Liquid**	**Liquid**
Temperature	**C**	117.864	30.000	35.000	55.599
Mass Flow	**kg/h**	401.000	420.000	401.000	420.000
Mass Fraction					
ACETI-01		0.998	0.000	0.998	0.000
SUCCI-01		0.000	0.000	0.000	0.000
ETHAN-01		0.000	0.000	0.000	0.000
WATER		0.002	1.000	0.002	1.000
MONOE-01		0.000	0.000	0.000	0.000
DIETH-01		0.000	0.000	0.000	0.000
ETHYL-01		0.000	0.000	0.000	0.000

XYLOS-01		0.000	0.000	0.000	0.000
Column 2 (SAC)					
		Input	**Output**	**Output**	
Phase		**Mixed**	**Liquid**	**Liquid**	
Temperature	**C**	100.594	107.863	90.601	
Mass Flow	**kg/h**	3461.798	661.798	2800.000	
Mass Fraction					
ACETI-01		0.000	0.000	0.000	
SUCCI-01		0.117	0.000	0.612	
ETHAN-01		0.091	0.113	0.000	
WATER		0.779	0.887	0.322	
MONOE-01		0.000	0.000	0.000	
DIETH-01		0.000	0.000	0.000	
ETHYL-01		0.000	0.000	0.000	
XYLOS-01		0.013	0.000	0.066	
Crystallizer					
		Input	**Output**	**Output**	
Phase		**Liquid**	**Mixed**	**Vapor**	
Temperature	**C**	107.863	135.000	135.000	
Mass Flow	**kg/h**	661.798	448.655	213.143	
Mass Fraction					
ACETI-01		0.000	0.000	0.000	
SUCCI-01		0.612	0.903	0.000	
ETHAN-01		0.000	0.000	0.000	
WATER		0.322	0.001	0.998	
MONOE-01		0.000	0.000	0.000	
DIETH-01		0.000	0.000	0.000	
ETHYL-01		0.000	0.000	0.000	
XYLOS-01		0.066	0.097	0.002	
Filtration Unit					
		Input	**Output**	**Output**	
Phase		**Mixed**	**Liquid**	**Solid**	
Mass Flow	**kg/h**	448.655	43.355	405.300	
Mass Fraction					
ACETI-01		0.000	0.000	0.000	
SUCCI-01		0.903	0.000	0.999	
ETHAN-01		0.000	0.000	0.000	
WATER		0.001	0.000	0.001	
MONOE-01		0.000	0.000	0.000	
DIETH-01		0.000	0.000	0.000	
ETHYL-01		0.000	0.000	0.000	
XYLOS-01		0.097	1.000	0.000	

Column 3 (Ethanol)					
		Input	**Output**	**Output**	
Phase		**Mixed**	**Liquid**	**Liquid**	
Temperature	**C**	90.843	78.200	100.014	
Mass Flow	**kg/h**	5745.000	675.000	5070.000	
Mass Fraction					
ACETI-01		0.001	0.000	0.001	
SUCCI-01		0.000	0.000	0.000	
ETHAN-01		0.109	0.926	0.000	
WATER		0.890	0.074	0.999	
MONOE-01		0.000	0.000	0.000	
DIETH-01		0.000	0.000	0.000	
ETHYL-01		0.000	0.000	0.000	
XYLOS-01		0.000	0.000	0.000	
HX2 (Ethanol)					
		Input	**Input**	**Output**	**Output**
Phase		**Liquid**	**Liquid**	**Liquid**	**Liquid**
Temperature	**C**	30.000	78.200	56.579	35.000
Mass Flow	**kg/h**	800.000	675.000	800.000	675.000
Mass Fraction					
ACETI-01		0.000	0.000	0.000	0.000
SUCCI-01		0.000	0.000	0.000	0.000
ETHAN-01		0.000	0.926	0.000	0.926
WATER		1.000	0.074	1.000	0.074
MONOE-01		0.000	0.000	0.000	0.000
DIETH-01		0.000	0.000	0.000	0.000
ETHYL-01		0.000	0.000	0.000	0.000
XYLOS-01		0.000	0.000	0.000	0.000

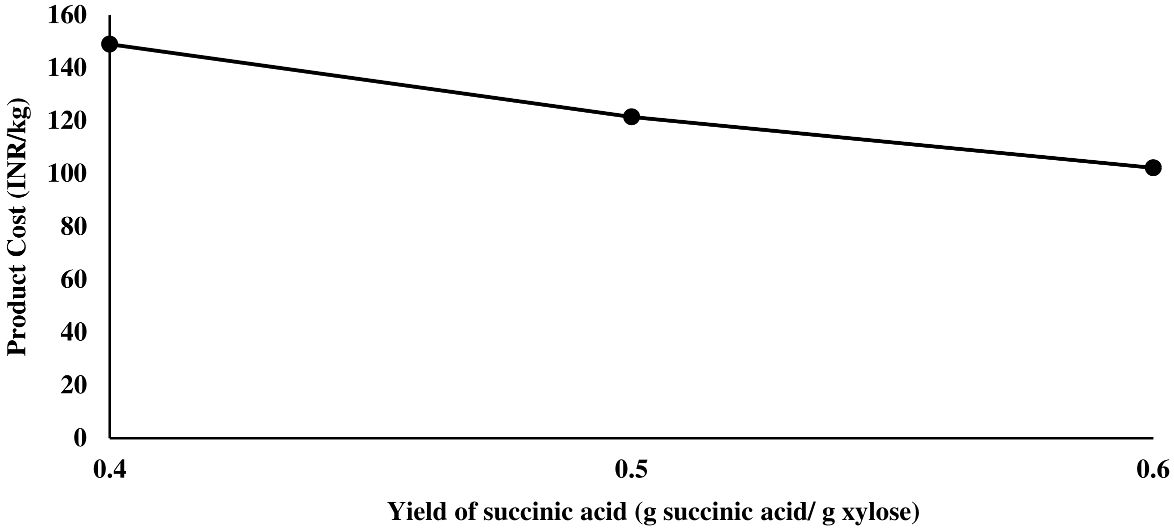

Figure S2: Impact of variation in yield of succinic acid in the fermentation stage on the product cost of succinic acid

Table S6: Impact of variation in yield of succinic acid in the fermentation stage on the economic parameters of the plant. Note that NPV and rate of return values are calculated if the selling price is kept at 178 INR/kg as determined for a four-year payback period for the base case yield of 0.5 g/g of xylose

Succinic acid yield (g succinic acid per g xylose)	**0.4**	**0.5**	**0.6**
Product cost (INR/kg)	149 ($ 1.73 /kg)	121 ($ 1.73 /kg)	102 ($ 1.73 /kg)
Rate of return (ROR)%	16.59	17.89	22.24
NPV (INR Million)	592 ($ 8.45 Million)	941 ($ 10.9 Million)	1,318 ($ 18.82 Million)
Raw material cost (INR Million)	11.77 ($ 0.168 Million)	11.82 ($ 0.168 Million)	11.82 ($ 0.168 Million)
Utilities cost (INR Million)	9.81 ($ 0.14 Million)	9.83 ($ 0.14 Million)	10.02 ($ 0.143 Million)
Purchased equipment cost (INR Million)	444 ($ 6.34 Million)	442 ($ 6.31 Million)	446 ($ 6.37 Million)

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