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Article

# Techno-Economic Analysis for the Production of 2,3-Butanediol from Brewers' Spent Grain Using Pinch Technology

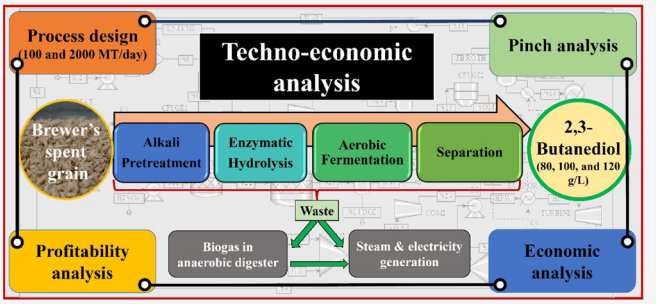
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**ABSTRACT:** 2,3-Butanediol (BDO) is a versatile platform chemical with great potential as the precursor for various value-added derivatives across different industrial sectors. This work thus presents a techno-economic feasibility study for microbial BDO production from $C_5$ and $C_6$ sugars derived from brewers' spent grain (BSG). Water-soluble carbohydrates obtained from pretreatment were further utilized for the biogas generation. Besides, the solid residue generated after fermentation and biogas were used to generate high-pressure steam and electricity. The process integration was carried out using pinch technology for various BDO titers and plant capacities. The pinch analysis helped in the reduction of hot and cold utility consumption by about 34 and 18%, respectively. The minimum hot and cold utility consumption was 4.59 and 10.97 MW for 100 MT BSG per day with 100 g/L BDO titer, respectively. The cooling water consumption was decreased, and electricity generation was increased with the increase in BDO titer, while the BDO production cost reduced marginally. For 100 MT BSG per day, the BDO production cost was US$1.84, US$1.76, and US$1.74/kg for BDO titers of 80, 100, and 120 g/L, respectively. However, the unitary BDO production cost was only US$1.07 for 2000 MT BSG per day. For 100 g/L BDO titer, the minimum BDO selling price was US$3.63 and US$2.00/kg for 100 and 2000 MT BSG per day, respectively, with 8.5% return on investment and 5 years as the payback period.



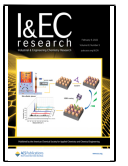

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## 1. INTRODUCTION

2,3-Butanediol (BDO) is a versatile bulk platform chemical with a vast range of applications in the food, cosmetic, and pharmaceutical industries. BDO derivatives, such as 1,3-butadiene, methyl ethyl ketone, and so forth, have strong commercial potentials.[1−3] For instance, 1,3-butadiene is an important monomer in synthetic rubber industries for the production of polybutadiene, styrene-butadiene, acrylonitrile-butadiene-styrene, and so forth. On the other hand, methyl ethyl ketone is a versatile solvent with a wide range of applications in the textile, plastic, cosmetics, and petroleum industries. Besides, BDO exhibits promising biofuel properties, such as high octane number and high heating value (26.8 MJ/L) superior to ethanol (23.4 MJ/L) and methanol (17.5 MJ/L) and similar to bio-butanol (26.78 MJ/L).[4,5] Therefore, BDO can be a potential fuel additive in gasoline engine. The high BDO titers (100−150 g/L) compared to bio-butanol (20−30 g/L) demonstrates the potential for commercial viability of microbial BDO production route.[6,7] Moreover, $C_8$−$C_{16}$ range hydrocarbon biofuels can be derived from BDO via an acid-catalyzed oligomerization reaction of butenes and hydrogenation of the resulting oligomers.[8] Downstream products of BDO have an estimated global market potential of around 32 million tons per annum, valued at US$43 billion.[9] Currently, BDO is produced industrially by the petrochemical route from 2-butylene via 2,3-epoxybutane. Petroleum is, however, finite and a non-renewable resource and depleting rapidly. The use of petroleum is also associated with long-term environmental implications. Therefore, the production of bio-based organic chemicals such as BDO has been emphasized in recent times for the sustainability of our planet.

BDO can be produced by various wild-type and genetically engineered microorganisms such as *Klebsiella* sp.,[10] *Enterobacter* sp.,[11] *Bacillus* sp.,[12] *Serratia* sp.,[13] *Panebacillus* sp.,[14] and *Saccharomyces cerevisiae*.[15] Most of the bacterial isolates reported for BDO production can utilize lignocellulose biomass-derived $C_6$ and $C_5$ sugars as the substrates.[16] In the last few decades, lots of work has been done on bio-based BDO production.[3] Despite all that, even today, the dominant route for the industrial manufacturing of BDO is the petrochemical one. The high cost of feedstock and expensive product recovery are largely contributing to the high

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manufacturing cost of BDO via the microbial route and impede industrial implementation.[1]

Waste generation is a global problem, and every year ∼3.7 billion tons of agricultural residues[17] and 1.3 billion tons of food residues[18] are generated worldwide. Beer manufacturing is a large-scale industry in several parts of the world, and brewer's spent grain (BSG) is the main byproduct in this process. In 2018, the annual beer production was 1.94 billion hectoliters which resulted in 38.8 million tons of BSG.[19,20] European Union is the second largest producer of beer, and ∼40 million tons of beer with 10.8 million tons of BSG were produced by European Union-28 countries in 2016. Among them, UK manufactured 5.15 million tons of beer annually with the co-generation of 194,000 tons of BSG.[21,22] BSG is a low-priced (∼US$50/ton) waste byproduct of breweries with a high amount of polysaccharides and proteins.[19] The nutritional rich value of BSG demonstrates its high biorefining potentials. Developing integrated biorefineries based on these biogenic residues rich in renewable and fermentable carbon would maximize the profit of breweries, minimize waste, and leads to the development of low-carbon biomanufacturing technologies with a circular economy approach.[22,23]

In our recent work, we have achieved a high level of BDO production (>100 g/L) using cellulosic glucose from BSG by *Enterobacter ludwigii*, a bacterium with a strong BDO manufacturing ability.[6] In another study, BDO accumulated on xylose-rich hydrolysate from sugarcane bagasse was efficiently separated using an aqueous-two phase system extraction, and the product recovery was >95%.[24] Contrary to bioethanol and bio-butanol, BDO does not form an azeotrope with water. The separation of BDO from the fermentation broth is thus much easier with lower capital investment and lesser energy consumption compared to bioethanol and bio-butanol.[25] The results on BDO accumulation and recovery are promising and demonstrate the potential for successful scale-up and commercialization. The titers and the strain efficiency in conversion of BSG to BDO determine the potential of industrial implementation. However, the feasibility of the process for the commercial-scale can be assessed by techno-economic evaluation in each stage of the process. In the recent past, Penner et al. modeled various separation methods for the dehydration of BDO obtained from the microbial fermentation process.[25] In another study, NREL reported the production of hydrocarbon biofuels and various products from lignocellulose biomass via BDO.[8] However, to the best of our knowledge, the techno-economic feasibility study for the conversion of BSG to BDO was not reported in the literature until now. Therefore, the main objective of this study was to evaluate the techno-economic feasibility and profitability for converting fermentable sugars obtained from BSG into BDO. The process involves alkali pretreatment of BSG, followed by enzymatic hydrolysis, aerobic fermentation, and separation of BDO from the fermentation broth. The process was designed based on the experimental results obtained previously.[6]

For any chemical manufacturing process, energy consumption is a vital operating cost-contributing factor. Energy saving is thus critical for improving the economic performance of the process. The pinch technology is an important process integration tool for energy saving, thereby improving the thermal efficiency of the process. In our work, process integration was carried out using the principle of pinch technology to minimize utility consumption. The simulations for mass and energy balances and process economic calculations were carried out using Aspen Plus software. A detailed analysis was further performed to identify the cost governing factors and effect of BSG price on the BDO production cost. The profitability analysis plays an important role in understanding the return on investment and will help to draw the attention of investors for possible investments. In this work, we performed the return on investment analysis to calculate the minimum BDO selling price for various returns on investment. The results of this study will eventually help out in predicting the prospects of the commercial viability for the biomanufacturing of BDO.

## 2. METHODOLOGY

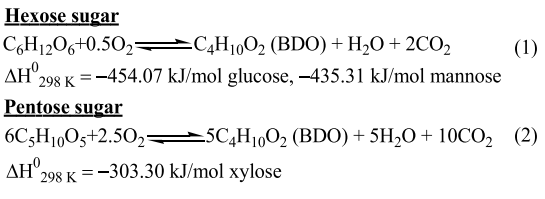
**2.1. Biomass Composition.** A wide variation in the BSG composition was reported in the literature. However, the present process design was carried out using a fixed dry composition of BSG as per the report of Meneses et al., 2013.[26] The composition of dry BSG is as follows: 21.73 wt % cellulose, 19.27 wt % hemicellulose (13.63 wt % xylan and 5.64 wt % glucomannan), 19.40 wt % lignin, 24.69 wt % proteins, 4.18 wt % ash, and 10.73 wt % extractives. Furthermore, the water content in the BSG was reported to vary excessively across many literature reports and considered 10 wt % in the current work. The cellulose was represented by the cellulose-R ($C_6H_{10}O_5$) segment with a degree of polymerization of 10,000 and a molecular weight of 1,621,424. The degree of polymerization of xylan was taken as 200. The glucomannan was composed of 200 dextran-R ($C_6H_{10}O_5$) segments with a molecular weight of 32,428.5. The lignin was considered solid with the molecular formula of $C_{7.3}H_{13.9}O_{1.3}$. The protein was represented by the molecular formula of $CH_{1.59}N_{0.24}O_{0.42}S_{0.01}$. The extractives generally represent non-structural components of the biomass, a portion of which accounts for mass balance closure, and the remaining portions comprise sugar alcohols and $C_4-C_6$ organic acids.[8] In our work, the extractives were represented by gluconic acid. The enzyme used in the hydrolysis of carbohydrates was represented by the molecular formula of $CH_{1.57}N_{0.29}O_{0.31}S_{0.007}$. The various physical properties of the non-conventional biomass components were obtained from the NREL databank.[27] The parameters of the various physical property models, such as liquid molar volume, solid volume, solid heat capacity, and vapor pressure, were first estimated using these property data. The processes were then designed using these fitted property models.

**2.2. BSG Processing Conditions.** The alkaline pretreatment of BSG was carried out under atmospheric pressure at 90 °C for a period of 1.5 h with 10 wt % biomass loading and 70 mg of NaOH per g dry BSG. During the alkaline pretreatment, some parts of the cellulose, hemicellulose, and lignin dissolve in water. In this work, we considered the dissolution of entire extractives, 47% lignin, 30% glucomannan, 10% xylan, and 2% cellulose, respectively.[8] The enzymatic hydrolysis of carbohydrates was carried out using mixed enzymes (cellulase and hemicellulase) at 50 °C for a period of 84 h with a protein (enzyme) loading of 10 mg per g carbohydrates.[8] We assumed 90% hydrolysis of carbohydrates during enzymatic treatment. The hydrolysis reactions are exothermic, releasing about −869.82 and −888.58 kJ per mole of glucose and mannose, respectively. The fermentation was carried out at 32 °C for a period of 72 h under aerobic conditions using air as a source of oxygen. We assumed 95% conversion of hydrolyzed sugars into BDO in the fermenter. In our process design, we considered


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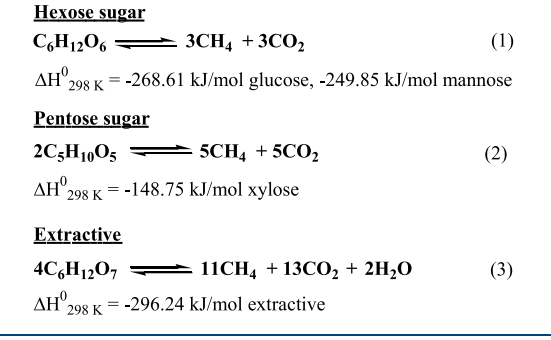
the simultaneous fermentation of both hexose and pentose sugars. The reaction stoichiometry for the aerobic fermentation of hexose and pentose sugars to BDO is shown in Scheme 1. The reaction stoichiometry shows a theoretical maximum

**Scheme 1. Reaction Stoichiometry for Aerobic Fermentation of Hexose and Pentose Sugars to BDO**




yield of 0.5 g BDO per g of both pentose and hexose sugars. Aerobic fermentation of sugars is also an exothermic reaction. The heat of reaction reported in Scheme 1 was calculated from Aspen Plus software. However, for the simplicity of the process design, the nutrient and inoculum needed for fermentation was not included in the process design. Nevertheless, the costs of nutrients (0.27 kg/kg BDO) and inoculum (1.43 kg/kg BDO) were included in the economic analysis. Due to the lack of suitable data, the amounts of nutrients and inoculum considered in current work were assumed to be similar to those of cellulosic bio-butanol production.[28] BDO accumulation through the biological route has been reported up to 150 g/L in the literature.[1] In our process design, a BDO titer of 100 g/L was considered as the base case. Furthermore, the BDO titer was varied from 80 to 120 g/L to exhibit its effect on the BDO manufacturing cost. The water-soluble organic stream (sugars, extractives, lignin, and NaOH) generated from the alkaline pretreatment step was first neutralized by sulfuric acid and then sent for anaerobic digestion (AD) for the biogas generation (Scheme 2). AD was carried out at 40 °C for a

**Scheme 2. Reaction Stoichiometry for Anaerobic Digestion**




period of 14 days. The biogas was composed of around 1:1 $CH_4/CO_2$ (mole). The lignin is, however, recalcitrant in nature and remains unreacted in AD. The unconverted fraction in AD was recovered as sludge that was composed of lignin (77%) and ash (23%) with a small amount of water. This sludge can be utilized as fertilizer.[29] The sludge credit of US $0.055 per kg (dry) was considered for economic analysis.[30] AD is an exothermic reaction. The heat of reactions reported in Scheme 2 was also calculated from Aspen Plus software. The solid residue recovered after fermentation and biogas obtained from AD were used to generate high-pressure steam. A part of the high-pressure steam was consumed in the process, and the excess high-pressure steam was utilized for generating electricity using the Rankine cycle.

**2.3. Techno-Economic Analysis.** The BDO production process was designed using Aspen Plus software (version 10) for a plant capacity of 100 MT BSG per day as a base case. On an average, 10.8 and 0.2 million tons of BSG was generated annually by breweries in the European Union and UK, respectively.[19] This scenario thus represents the decentralized processing of BSG to avoid its expensive transportation to a faraway centralized facility. However, the production cost is known to decrease with the increase in plant capacity for any chemical manufacturing processes. Therefore, the techno-economic performance of base case plant capacity was compared with 2000 MT BSG per day plant capacity. This plant capacity represents the centralized processing of BSG. The centralized biorefinery, however, involves the transportation of BSG from far away breweries. The BSG transportation cost was calculated considering 500 km as the average distance of centralized processing plants from breweries. BSG was assumed to be transported by trucks with a maximum loading capacity of 26 MT and fuel (2.09 US $/L) consumption of 0.3 L/km.[31] Based on the fuel consumption, the transportation cost of BSG was found to be US$12.07/MT. Additionally, the labor costs, including loading and unloading, were taken as US$6.7/MT.[32] The total cost of transportation and labor (US$18.77/MT) was added to the base price of BSG for economic analysis in a centralized biorefinery.

Economic analysis was performed considering 10 years as the plant life with 8760 h as the working hour per annum. The cost of the equipment with different sizes (B) was calculated using the cost of the same equipment with known size (A) by the following equation.[33]

$$\text{Cost of equipment B} = \text{cost of equipment A} \times \left(\frac{\text{size of equipment B}}{\text{size of equipment A}}\right)^{0.6}$$

The hydrolysis reactor and fermenter costs were, however, calculated based on the numbers of 500 $m^3$ (or 250 $m^3$) reactors. For 100 MT BSG per day plant capacity, 2.5, 2, and 2 hydrolysis reactors were needed for BDO titers of 80, 100, and 120 g/L, respectively. The fermentation was carried out using 2, 1.5, and 1.5 reactors for BDO titers of 80, 100, and 120 g/L, respectively. For 2000 MT BSG per day plant capacity, 39 hydrolysis reactors and 27 fermenters were considered for the economic analysis. In our economic analysis, we considered the storage tanks for maintaining 12 and 25 days stocks of chemicals and BDO, respectively. The storage tank cost was calculated considering US$80 as the storage cost per barrel. The direct fixed costs include installation, instrumentation and control, piping, electrical, building, yard improvement, service facilities, and land. These costs were taken as 52, 30, 75, 12, 20, 11, 77, and 5% of total equipment cost, respectively.[34] The indirect fixed costs include engineering and supervision, construction expenses, legal expenses, contractor fees, and contingency and were taken as 9, 11, 1, 6, and 12% of direct fixed cost, respectively.[34,35] The working capital was taken as 5% of the total fixed capital cost.

The operating costs consist of direct and indirect costs. The labor and maintenance, operating and plant overhead charges, utilities, raw materials, and chemicals were included in the direct costs. The price of BSG, chemicals, and utilities considered in this techno-economic feasibility study was


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obtained from the literature, as shown in Table 1. For 100 MT BSG per day, the expenditure for operating labor was

**Table 1. Cost of BSG, Chemicals, and Utilities**

| | |
|---|---|
| BSG, US$/ton | 50 |
| process water, US$/kg | 0.00053 |
| cooling water, US$/1000 L | 0.032 |
| NaOH, US$/kg | 0.135[39] |
| $H_2SO_4$, US$/kg | 0.039[28] |
| enzymes, US$/kg | 2.359[39] |
| nutrient medium, US$/kg | 0.204[28] |
| inoculum, US$/kg | 0.006[28] |
| electricity, US$/kW h | 0.077 |
| sludge, US$/kg | 0.055[30] |
| steam@100 psi, US$/kg | 0.018 |

estimated considering one supervisor and four operators per shift with individual salaries of US$35 and US$20/h, respectively.[36] One supervisor with seven operators per shift was, however, considered for 2000 MT BSG per day. The indirect costs include depreciation of equipment, interest on the capital investment, insurance, and taxes. The depreciation of equipment was calculated using a straight-line method with 20% of the equipment cost as salvage value. The insurance and taxes were taken as 1.5% of the equipment cost.[34,35] In our economic analysis, the entire capital expenditure was borrowed from a bank with an annual interest rate of 5.5%. The chemical engineering plant cost index of 599.5 for the year 2020 was used to calculate the cost of equipment.[37] Profitability analysis was carried out using the price escalation factor of 5 and 3.5% for products and raw materials, respectively. However, 3% price appreciation was assumed for utility, maintenance, and operating labor.

**2.4. Pinch Analysis.** The pinch technology is an excellent process heat energy integration tool and aids efficient utilization of heat energy within the process. This analysis guides the effective design of the heat exchanger network by minimizing the consumption of external utility. For pinch analysis, the supply and target temperature, enthalpy change, and mass flow rate of process streams were extracted from the designed flowsheets. Moreover, the various unit operations either generate or consume heat and the heat duty involved in these unit operations was also extracted from the designed flowsheets. The unit operations are generally operated under isothermal conditions. However, for pinch analysis, 1 °C temperature difference between inlet and outlet was considered. The heat capacity flow rate was then calculated for each of the process streams and unit operations, and pinch analysis was then carried out using 10 °C as the minimum temperature difference. The minimum (cold and hot) utility consumption and pinch temperature were calculated from the composite and grand composite curve. The design of heat exchangers was then carried out for the maximum process heat recovery based on the principle of pinch technology. The cold water and high-pressure steam were used as the cold and hot utility, respectively.

## 3. RESULTS AND DISCUSSION

**3.1. Process Design.** At first, BSG was grinded using dry milling (Figure 1). The grinded BSG was then sent for alkaline pretreatment. Simultaneously, water containing a required quantity of NaOH was preheated to 90 °C and directed to the pretreatment reactor. In general, BSG generated in the brewery contains about 70−80% water.[19] For the processing of BSG in a decentralized biorefinery close to the brewery, the energy-intensive drying of wet BSG can be avoided with minimal or no addition of water for pretreatment. The biomass slurry obtained from the pretreatment was cooled to 50 °C. The solid biomass obtained from the pretreatment was separated using a centrifuge and sent for hydrolysis. The quantity of water added in the hydrolysis reactor was based on the desired BDO titer in

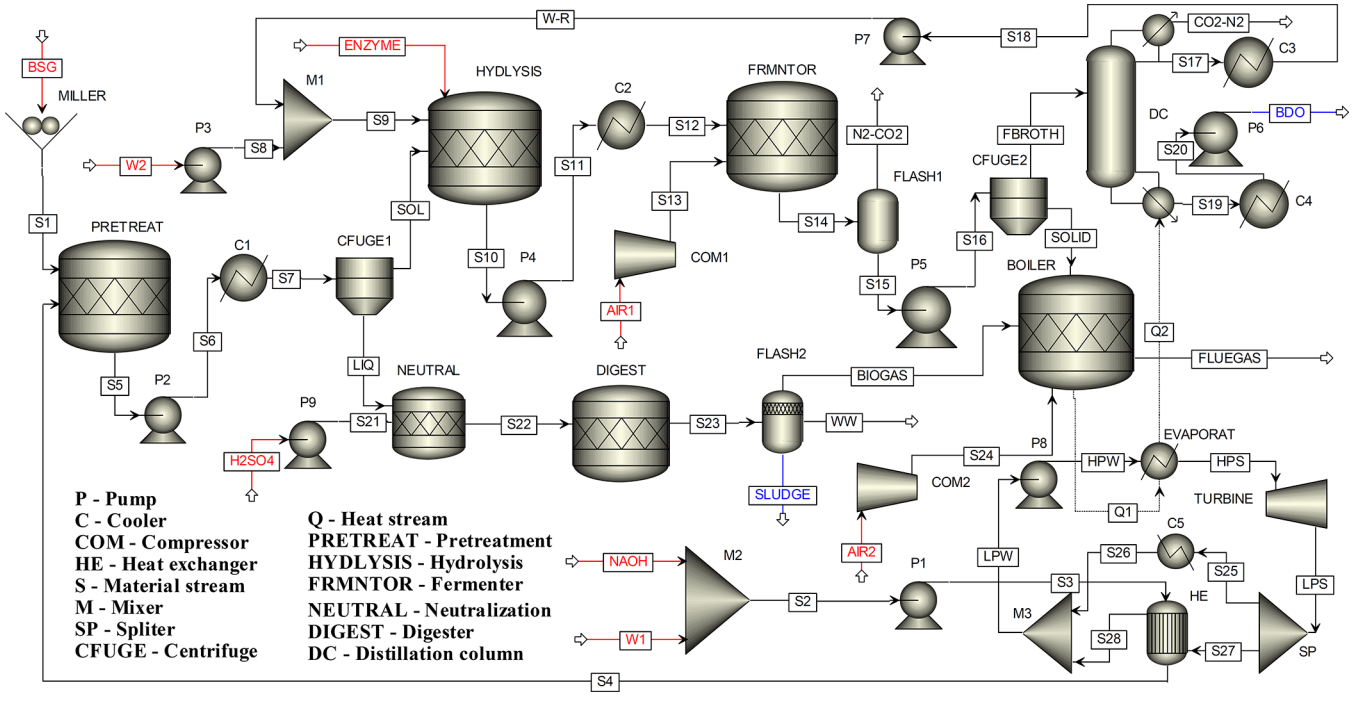



**Figure 1.** Heat-integrated process flowsheet for the bioproduction of BDO from BSG.



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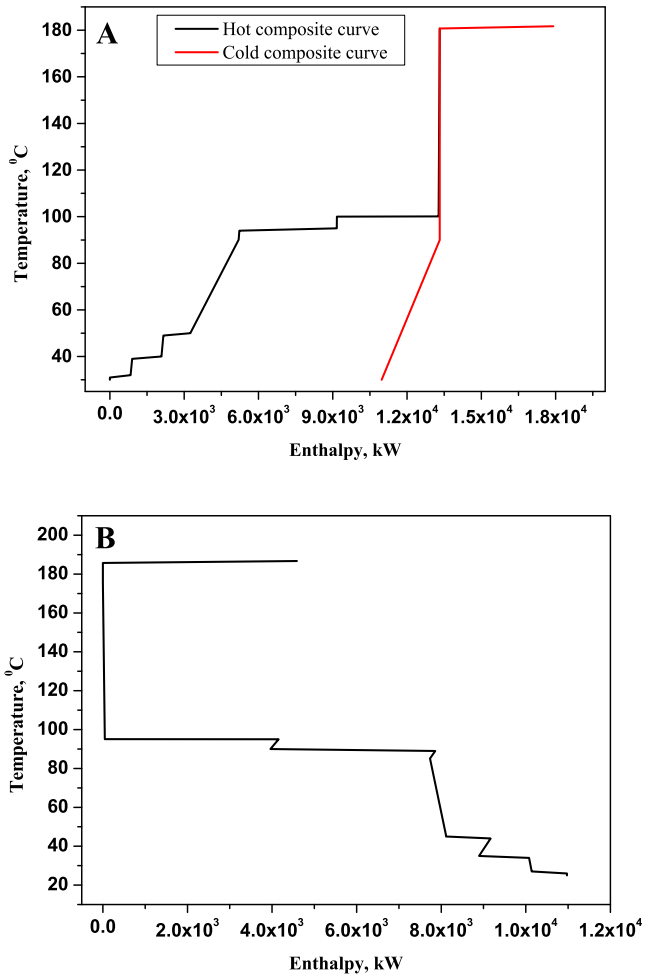



**Figure 2.** (A) Composite and (B) grand composite curve for plant capacity of 100 MT BSG per day with BDO titer of 100 g/L.

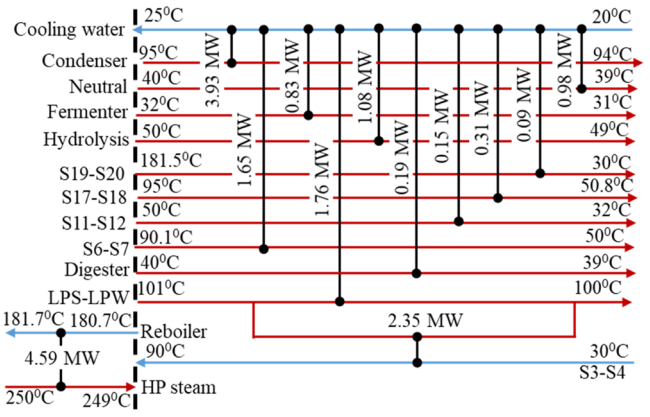



**Figure 3.** Grid diagram for the heat exchanger network design for plant capacity of 100 MT BSG per day with BDO titer of 100 g/L in fermentation.

the fermentation. The total sugar concentrations required for 80, 100, and 120 g/L BDO titers were about 186, 240, and 297 g/L, respectively. Both pretreatment and hydrolysis units were modeled using the RStoic reactor (Scheme 1). The sugar solution obtained from the hydrolysis reactor was cooled to 32 °C and then directed to the fermenter. Fermentation was carried out using a continuous flow of air with a constant venting out of carbon dioxide and nitrogen from the reactor.

**Table 2. Consumption of Utility and Chemicals and Cogeneration of Sludge and Electricity**

| | 100 MT BSG per day | | | 2000 MT BSG per day |
|---|---|---|---|---|
| | 80 g BDO/L | 100 g BDO/L | 120 g BDO/L | 100 g BDO/L |
| cooling water, MT/annum | $1.76 \times 10^7$ | $1.72 \times 10^7$ | $1.50 \times 10^7$ | $3.35 \times 10^8$ |
| process water, MT/annum | | $2.94 \times 10^5$ | | $5.87 \times 10^6$ |
| $H_2SO_4$, MT/annum | | $2.82 \times 10^3$ | | $5.64 \times 10^4$ |
| NaOH, MT/annum | | $2.30 \times 10^3$ | | $4.60 \times 10^4$ |
| enzyme, MT/annum | | $1.23 \times 10^2$ | | $2.46 \times 10^3$ |
| nutrients, MT/annum | | $1.68 \times 10^3$ | | $3.35 \times 10^4$ |
| inoculum, MT/annum | | $8.88 \times 10^3$ | | $1.78 \times 10^5$ |
| sludge, MT/annum | | $3.96 \times 10^3$ | | $7.93 \times 10^4$ |
| electricity consumed, MW | 0.30 | 0.30 | 0.30 | 3.04 |
| electricity generated, MW | 1.25 | 1.61 | 1.84 | 32.14 |
| net electricity generated, MW | 0.95 | 1.31 | 1.54 | 29.10 |

The aeration rate was 225.77 $m^3$/min (537.45 kmol/h) for 100 MT BSG per day plant capacity. In this work, the fermenter was modeled using the combination of the RStoic reactor and Flash2 separator. The Flash2 drum operated at 32 °C was used to separate carbon dioxide and nitrogen from the fermentation broth. The bottom stream from the Flash2 drum was centrifuged to separate solids (lignin, unconverted carbohydrates, and protein) from the fermentation broth, and the obtained solid was sent to the boiler to generate high-pressure steam. The fermentation broth was sent to the downstream separation of BDO from water by distillation. The distillation column (DC) was designed at atmospheric pressure using the RadFrac model with NRTL as the property method. The fermentation broth contains a small quantity of dissolved carbon dioxide and nitrogen. These gases were removed from the partial condenser of the DC. The condenser was operated at a subcooled temperature (95 °C) to reduce water loss with the gaseous stream. The capital investment and operating cost of the DC generally increase with the increase in number of stages and reflux ratio, respectively. The number of stages and reflux ratio were thus optimized by minimizing the following function ($f$): $f$ = (number of stages) × (reflux ratio). The DC was optimized to obtain more than 99.9% BDO recovery from the bottom of the DC. The feed stage location was identified by maximizing the purity of the distillate and bottom product. The optimum numbers of stages, feed tray location, and mass reflux ratio were 14, 10, and 0.061, respectively. The low reflux ratio was due to the large volumetric flow rate of water as distillate. The BDO obtained from the bottom of the DC was cooled to room temperature (30 °C) and then pumped to the storage tank. The yield of BDO was around 0.16 kg per kg of dry BSG. The water obtained as the distillate from the DC was cooled to 50.8 °C and recycled to the hydrolysis reactor.


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Table 3. Capital expenditure in Million US$

| plant capacity, MT/day | 100 | 100 | 100 | 2000 |
|---|---|---|---|---|
| BDO titer in fermentation, g/L | 80 | 100 | 120 | 100 |
| Miller | 0.184 | 0.184 | 0.184 | 0.789 |
| pretreatment | 0.111 | 0.111 | 0.111 | 0.486 |
| hydrolysis | 0.839 | 0.631 | 0.631 | 12.304 |
| fermenter | 0.631 | 0.524 | 0.524 | 8.518 |
| centrifuges | 0.840 | 0.840 | 0.840 | 10.924 |
| distillation column | 0.317 | 0.269 | 0.236 | 4.444 |
| neutralization reactor | 0.110 | 0.110 | 0.110 | 0.666 |
| anaerobic digester | 1.501 | 1.501 | 1.501 | 9.057 |
| compressors | 0.382 | 0.382 | 0.382 | 2.537 |
| boiler | 0.262 | 0.262 | 0.262 | 2.470 |
| turbine | 0.915 | 1.063 | 1.155 | 6.415 |
| pumps | 0.090 | 0.090 | 0.091 | 0.215 |
| heat exchangers | 0.079 | 0.089 | 0.095 | 0.380 |
| storage tanks | 0.222 | 0.222 | 0.222 | 4.448 |
| **total equipment cost** | **6.485** | **6.280** | **6.345** | **63.654** |
| installation | 3.372 | 3.266 | 3.299 | 33.100 |
| instrumentation and controls | 1.945 | 1.884 | 1.903 | 19.096 |
| piping | 4.864 | 4.710 | 4.759 | 47.740 |
| electricals | 0.778 | 0.754 | 0.761 | 7.638 |
| building | 1.297 | 1.256 | 1.269 | 12.731 |
| yard improvements | 0.713 | 0.691 | 0.698 | 7.002 |
| service facilities | 4.993 | 4.836 | 4.885 | 49.013 |
| land | 0.324 | 0.314 | 0.317 | 3.183 |
| **direct fixed cost ($a$)** | **24.772** | **23.990** | **24.237** | **243.157** |
| engineering and supervision | 2.230 | 2.159 | 2.181 | 21.884 |
| construction expenses | 2.725 | 2.639 | 2.666 | 26.747 |
| legal expenses | 0.248 | 0.240 | 0.242 | 2.432 |
| contractor fees | 1.486 | 1.439 | 1.454 | 14.589 |
| contingency | 2.973 | 2.879 | 2.908 | 29.179 |
| **indirect fixed cost ($b$)** | **9.661** | **9.356** | **9.452** | **94.831** |
| fixed capital cost ($c = a + b$) | 34.434 | 33.347 | 33.689 | 337.988 |
| working capital ($d$) | 1.722 | 1.667 | 1.684 | 16.899 |
| **total capital investment ($c + d$)** | **36.155** | **35.014** | **35.374** | **354.887** |

The water-soluble biomass obtained from the pretreatment was sent to the neutralization reactor, where NaOH was neutralized using $H_2SO_4$. The neutralization reactor was operated at 40 °C and modeled using the RStoic model. The neutralized solution was sent to the AD, where the biogas (1:1 methane/carbon dioxide) was produced. The biogas generated in the anaerobic digester was continuously removed from AD reactor and sent to the boiler. The anaerobic digester was modeled using a combination of RStoic reactor and Flash2 separator. The unconverted lignin and ash were separated from the bottom of the Flash2 drum. The solid biomass obtained after fermentation and biogas were combusted by air in the boiler to generate high-pressure steam (30 bar). The excess high-pressure steam was utilized for the generation of electricity using the Rankine cycle. The Rankine cycle was modeled using IAPWS-95 as the property method. The Flash1 and Flash2 drums are an intrinsic part of the fermenter and AD, respectively. The cost of these drums was thus not included in the economic analysis.

**3.2. Process Integration and Utility Consumption.** Two cold streams were involved in this process: aqueous NaOH (S3−S4) and reboiler of the DC. All the remaining process streams, including the condenser of the DC, were hot streams in this process. Furthermore, the heat energy was generated in the hydrolysis reactor, fermenter, neutralization reactor, and AD. These unit operations were thus considered as the hot streams. The composite and grand composite curve showed 175.7 °C as the shifted pinch point temperature in this process, that is, hot and cold side pinch point temperatures were 180.7 and 170.7 °C, respectively (Figure 2). Only the reboiler of the DC was above the pinch point temperature, while the remaining all process streams and unit operations were below it. Without process heat recovery, the total hot and cold utility consumption in the process was 6.94 and 13.32 MW, respectively, for the plant capacity of 100 MT BSG per day with a BDO titer of 100 g/L. However, the grand composite curve showed a significant scope of heat recovery (2.35 MW) within the process. Therefore, following the pinch analysis, the minimum hot and cold utility consumption was 4.59 and 10.97 MW, respectively. These results demonstrated that the pinch analysis helped to reduce hot and cold utility consumption by more than 34 and 18%, respectively.

Figure 3 shows the grid diagram for the design of the heat exchanger network, considering maximum process heat recovery for the plant capacity of 100 MT BSG per day with a BDO titer of 100 g/L. The low-pressure steam generated from the turbine (LPS) was split into two streams. One of the streams was used to heat the aqueous NaOH stream (S3) from room temperature to 90 °C. The other low-pressure stream and all the other hot streams were cooled using cooling water. Some part of the high-pressure steam was used to meet the heat duty of the reboiler in the DC. The excess high-pressure steam was utilized for the generation of electricity using the Rankine cycle (Table 2). The heat-integrated process flowsheet is shown in Figure 1.

The consumption of utility and chemicals and co-generation of sludge and electricity for various BDO titers and two different plant capacities are shown in Table 2. The cooling water consumption was reduced slightly with the increase in BDO titers. It was due to a decrease in the heat duty of the condenser in the DC. The heat duty of the reboiler was also dropped for higher BDO titers. The reduced reboiler duty, in turn, resulted in the diversion of an increased quantity of high-pressure steam to the Rankine cycle with the generation of a larger quantity of low-pressure steam. Because the heat duty of the aqueous NaOH stream (S3) remained unchanged, the net cooling duty for the low-pressure steam was increased with the reduction of reboiler duty. However, the decrease of cooling duty in the condenser was much higher compared to the increase in the net cooling duty for the low-pressure steam. Therefore, the consumption of cooling water was lower at higher BDO titers in fermentation. The electricity consumption in the process was practically similar for all three BDO titers. However, the electricity generation by the Rankine cycle was augmented for higher BDO titers. At an elevated BDO titer, the reboiler heat duty was decreased with reduced consumption of high-pressure steam. The net amount of high-pressure steam diverted to the Rankine cycle was thus increased for elevated BDO titer with the higher electricity generation. The water recovered in the DC was recycled to the hydrolysis reactor. Only a small quantity of makeup water was thus needed for hydrolysis to supplement the water loss in the flash drum and gaseous stream from the partial condenser. The process water consumption was thus practically identical for all BDO titers in fermentation. The consumption of $H_2SO_4$,


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Table 4. Operating Cost in Million US$ per Annum with and without Pinch Analysis

| plant capacity, MT/day | 100 | 100 | 100 | 2000 |
|---|---|---|---|---|
| BDO titer in fermentation, g/L | 80 | 100 | 120 | 100 |
| | | Direct Cost | | |
| operating labor | 1.007 | 1.007 | 1.007 | 1.533 |
| maintenance | 2.169 | 2.101 | 2.122 | 21.293 |
| operating charges | 0.252 | 0.252 | 0.252 | 0.383 |
| plant overhead charges | 1.588 | 1.554 | 1.565 | 11.413 |
| cooling water | 0.566 | 0.550 | 0.481 | 10.719 |
| BSG | 1.825 | 1.825 | 1.825 | 36.500 |
| feedstock transportation | - | - | - | 13.702 |
| process water | 0.156 | 0.156 | 0.156 | 3.115 |
| $H_2SO_4$ | 0.110 | 0.110 | 0.110 | 2.199 |
| NaOH | 0.310 | 0.310 | 0.310 | 6.209 |
| enzyme | 0.291 | 0.291 | 0.291 | 5.814 |
| nutrients | 0.342 | 0.342 | 0.342 | 6.837 |
| inoculum | 0.053 | 0.053 | 0.053 | 1.065 |
| | | Indirect Costs | | |
| insurance and taxes | 0.097 | 0.094 | 0.095 | 0.955 |
| depreciation | 0.519 | 0.502 | 0.508 | 5.092 |
| interest | 1.989 | 1.926 | 1.946 | 19.519 |
| general and administration expenses | 0.447 | 0.437 | 0.434 | 3.627 |
| **total operating cost** ($a$) | **11.722** | **11.511** | **11.497** | **149.976** |
| electricity credits ($b_1$) | −0.643 | −0.894 | −1.041 | −19.629 |
| sludge credit ($b_2$) | −0.218 | −0.218 | −0.218 | −4.362 |
| BDO produced, MT/annum ($c$) | 5896.8 | 5896.8 | 5896.8 | 117889.7 |
| | | With Pinch Analysis | | |
| net production costs ($d = a + b_1 + b_2$) | 10.861 | 10.399 | 10.238 | 125.986 |
| **production cost**, US$ per kg ($d/c$) | **1.842** | **1.764** | **1.736** | **1.069** |
| | | Without Pinch Analysis | | |
| additional utility ($e$) | 0.768 | 0.768 | 0.768 | 15.366 |
| net production costs ($f = d + e$) | 11.630 | 11.168 | 11.006 | 141.351 |
| **production cost**, US$ per kg ($f/c$) | **1.972** | **1.894** | **1.866** | **1.199** |

NaOH, enzyme, nutrients, and inoculum were, however, identical for all three BDO titers in fermentation.

**3.3. Capital Expenditure and Production Cost.** Anaerobic digester, hydrolysis reactor, fermenter, turbine, centrifuges, and DC were the major capital-intensive equipment and costing significantly to the process (Table 3). The high cost for the anaerobic digester was due to the large equipment size needed to run for a long residence time. The equipment cost for the hydrolysis reactor, fermenter, and DC was decreased slightly with the increase in BDO titer in fermentation due to the reduced volumetric flow rate with a smaller equipment size. However, the equipment cost for the heat exchanger and turbine was increased slightly with the increase in BDO titer in fermentation. With the increase in BDO titer in fermentation, reboiler heat duty was decreased with reduced steam consumption. As a result, a larger quantity of steam was diverted to the power generation cycle. The equipment cost of the above units was thus increased slightly as BDO titer was enhanced. However, the increase in capital investment for the heat exchanger and turbine was practically compensated by the reduction in equipment cost for the hydrolysis reactor, fermenter, and DC. The total capital investment was thus almost similar for all three BDO titers. The operating cost for the cooling water was, however, decreased and net electricity credit was increased at higher BDO levels (Table 2). The BDO production cost was thus decreased slightly as BDO concentration was increased (Table 4). However, the decrease in the BDO production cost was only about 5.75% for increasing the BDO titer from 80 to 120 g/L. On the other hand, for the 20-time increase in plant capacity from 100 MT per day to 2000 MT per day, both the total equipment cost and total capital investment were increased by about 10.14-fold only. This disproportionate increase in the total capital investment led to substantial drop in BDO production cost (US$1.07/kg) for the plant capacity of 2000 MT per day (Table 4). The BDO production cost was reported as 25.6 cents per pound of BDO according to 1952 year prices for a 60,000 pounds of molasses per day plant capacity.[38] Without process integration using pinch technology, the additional amount of cooling water and low-pressure steam was required to meet the heat duty for all process stream and unit operations (Table 4). The BDO production cost was thus slightly higher for the processes without heat integration. As observed from the Table 4, the process integration using pinch technology potentially reduced the BDO production cost by about 6.6−6.98 and 10.84% for 100 and 2000 MT BSG per day plant capacity, respectively. These results clearly demonstrate the importance of pinch analysis for process integration.

**3.4. Cost-Contributing Factors.** Figure 4A shows the various factors contributing towards the BDO production cost for the heat-integrated process using pinch technology. The direct cost was the major contributing factor for the 100 MT BSG per day plant capacity and contributed around 46−48% of BDO manufacturing cost. However, the contribution of the direct cost was reduced to around 27% of the BDO



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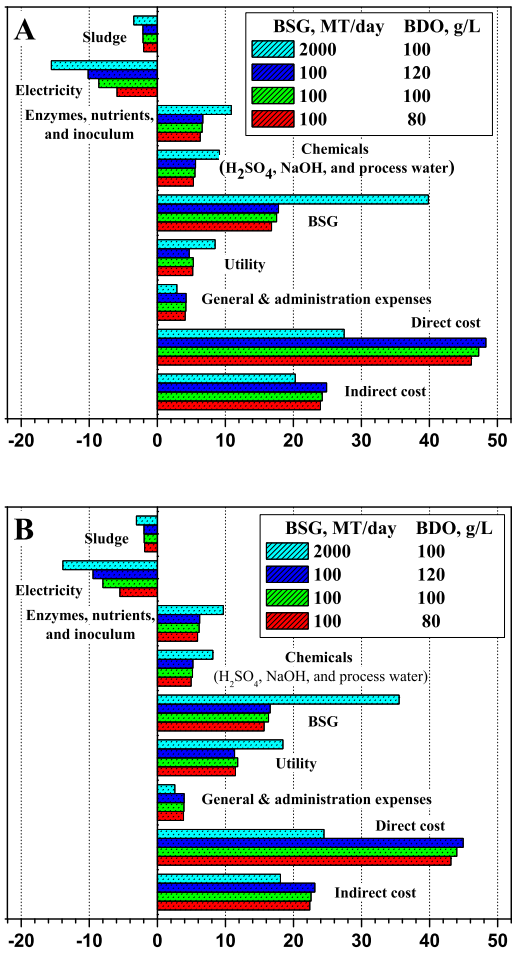



**Figure 4.** Cost-contributing factors for BDO production from BSG (A) with and (B) without pinch analysis.

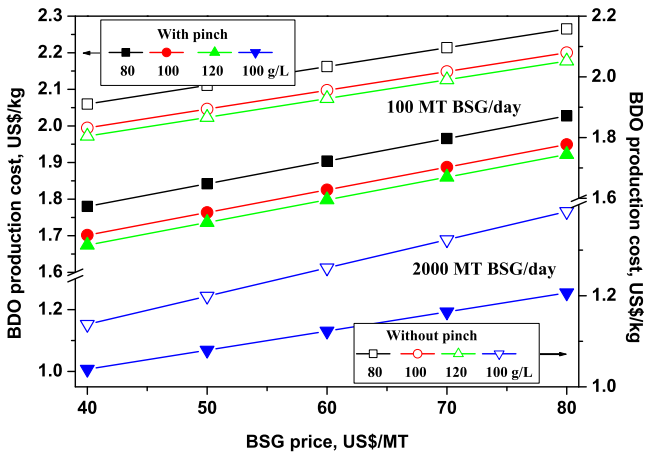



**Figure 5.** Effect of price of BSG on the BDO production cost.

manufacturing cost for the 2000 MT BSG per day plant capacity. It was due to the disproportionate increase in the total capital investment with the increase in plant capacity. The feedstock (BSG) contributed only about 16.8−17.8% of the BDO production cost for 100 MT BSG per day plant capacity. However, the contribution of BSG was around 39.8% of the BDO production cost for 2000 MT BSG per day plant capacity. It was due to the reduction in the contribution of the direct cost on the BDO production cost. The contribution of

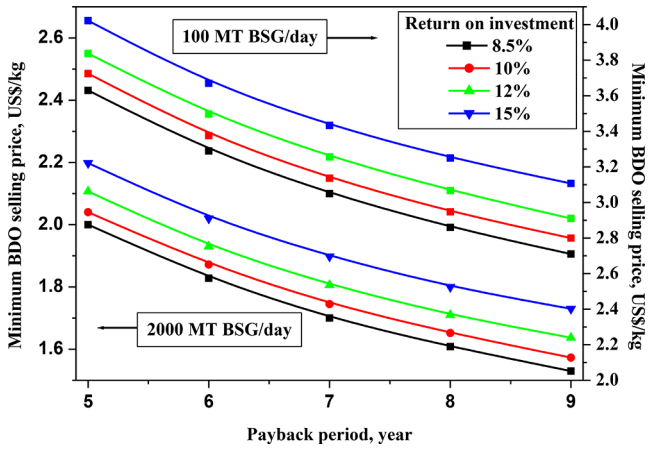



**Figure 6.** Return on investment analysis using economic analysis data based on pinch analysis for 100 g/L BDO titer achieved during fermentation.

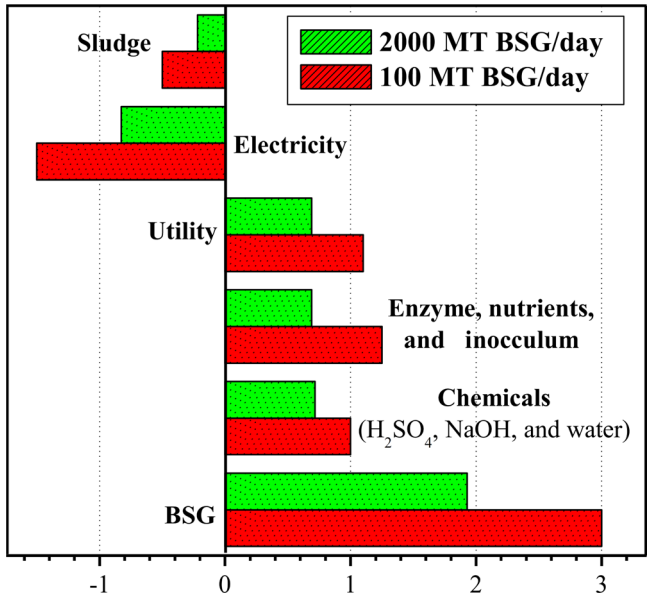



**Figure 7.** Percentage change in minimum BDO selling price for +20% rise in the price of various factors with BDO titer of 100 g/L.

the indirect cost was nearly 20−25% of the BDO manufacturing cost for both plant capacities. The electricity credit (around 16%) was significant for 2000 MT BSG per day plant capacity. For 100 MT BSG per day plant capacity, electricity credit was only around 5.9% for 80 g/L BDO titer and increased to about 10.2% of the production cost for 120 g/L BDO titer. The sludge contributed around 2−3.5% of the production cost. The contribution of chemicals, general and administrative expenses, and enzymes, nutrients, and inoculum were in the range of 5−9, 3−4, and 6−11% of the production cost, respectively. For 100 MT BSG per day plant capacity, the contribution of both direct and indirect cost was increased slightly with the increase in BDO titer in the fermentation. It was due to the increase in electricity credit with the increase in BDO titer in the fermentation. Without process integration using pinch technology, the contribution of the utility on the production cost was quite significant for both 100 MT (11−12%) and 2000 MT (18%) BSG per day plant capacity (Figure 4B). Following the pinch analysis, the contribution of the


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utility on the BDO production cost was reduced to only about 5 and 8.5% for 100 MT and 2000 MT BSG per day plant capacity, respectively (Figure 4A).

**3.5. Effect of the Price of BSG on the BDO Production Cost.** The BSG price is sensitive to the geographical origin. Thus, the BSG price was varied to see its influence on the BDO production cost for both with and without process integration using pinch technology, as shown in Figure 5. For a 25% escalation in the BSG price from US$40 to US$50 per MT, the unitary BDO production cost was increased by about 3.47−3.69 and 6.15% with pinch analysis and 3.24−3.43 and 5.45% without pinch analysis for 100 MT and 2000 MT BSG per day plant capacity, respectively. The higher escalation in the BDO production cost for 2000 MT BSG per day plant capacity was due to the greater contribution of feedstock on the BDO production cost (Figure 4). For the price of US$80 per MT of BSG, the unitary BDO production cost was found to be around US$1.92−2.03 and US$1.25 with pinch analysis and US$2.05−2.16 and US$1.38 without pinch analysis for the plant capacity of 100 MT and 2000 MT BSG per day, respectively.

**3.6. Profitability Analysis.** Profitability analysis was carried out for the heat integrated processes with 100 and 2000 MT BSG plant capacity and 100 g/L BDO titer in fermentation (Figure 6). Return-on-investment analysis was carried out to obtain the minimum BDO selling prices for the payback period in the range of 5−9 years and the return on investment in the range of 8.5−15%. The minimum selling price is defined as the price of BDO at which the net present value of all future cash flows becomes zero for a specific payback period and a fixed return on investment. The selling price generally includes sales tax, which is country specific. Therefore, in the present profitability analysis, the sales tax was not included in the minimum BDO selling price. The minimum BDO selling price was decreased with the increase in payback period and decrease in return on investment. For 100 MT BSG per day plant capacity with 5 years as a payback period, the minimum selling price per kg of BDO was US$3.63 for 8.5% return on investment and increased to US$4.02 for 15% return on investment. The minimum selling price per kg of BDO was reduced to US$2.71 and US$3.11 for 8.5 and 15% return on investment, respectively, with payback period of 9 years. For 2000 MT BSG per day plant capacity with 5 years as a payback period, the minimum selling price per kg of BDO was US$2.00 for 8.5% return on investment and increased to US$2.20 for 15% return on investment which dropped to US $1.53 and US$1.73 for 8.5 and 15% return on investment, respectively, when payback period was increased to 9 years. For 100 MT BSG per day plant capacity with 5 years as a payback period, the selling price per kg of BDO with 20% sales tax was US$4.36 and US$4.82 for 8.5 and 15% return on investment, respectively, while it reduced to US$2.40 and US $2.64 for 8.5 and 15% return on investment, respectively, for 2000 MT BSG per day plant capacity with 5 years as a payback period. The current BDO price is about US$3.23 per kg.[14] These results demonstrate that the selling price of microbial BDO after the addition of sales taxes in a centralized facility is quite competitive with the current price of BDO obtained from the petrochemical route even with a short payback period (5 years) and high return on investment (15%). However, the decentralized microbial production of BDO from BSG is slightly expensive compared to petrochemical BDO. The sensitivity analysis was further performed to understand the effects of various factors on the minimum BDO selling price, as shown in Figure 7. The analysis was performed for +20% rise in the price of various factors for 8.5% return on investment and 5 years as a payback period. The minimum BDO selling price was increased by around 3 and 2% for 20% increase in feedstock cost for 2000 and 100 MT BSG plant capacity, resectively. However, the minimum BDO selling price change was around 1% or below 1% for 20% rise in the price of all other factors.

## 4. CONCLUSIONS

The current study demonstrated the techno-economic feasibility of microbial BDO production from BSG using pinch technology. The pinch analysis helped in the reduction of the hot and cold utility consumption in the process that ultimately lowered the BDO manufacturing cost. The capital investment was almost identical at all BDO titers for a fixed plant capacity. However, decrease in cooling water and increase in electricity generation was observed at higher BDO titers. The production cost was thus slightly lower for higher BDO titers. The BDO production cost was significantly higher for 100 MT BSG per day (US$1.74−1.84/kg) compared to 2000 MT BSG per day (US$1.07/kg). The BSG price contributed about 16.8−17.8 and 39.8% to the BDO manufacturing cost, while the direct cost contributed around 46−48 and 27% for 100 and 2000 MT BSG per day, respectively. For 100 g/L BDO titer, the minimum selling price per kg of BDO was US$3.63 and US$2.00 for 100 and 2000 MT BSG per day with 8.5% return on investment and 5 years as the payback period, respectively. These results indicates the economical feasibility of microbial production of BDO from BSG in a large-scale centralized facility. Future work will be directed at environmental perfoermance of bioprocess using a cradle-to-factory gate life cycle assessment approach.

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‖S.M. and V.N. first author contribution




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## Notes

The authors declare no competing financial interest.

## ■ ABBREVIATIONS

AD anaerobic digestion
BSG brewers' spent grain
BDO 2,3-butanediol
DC distillation column
MT metric ton

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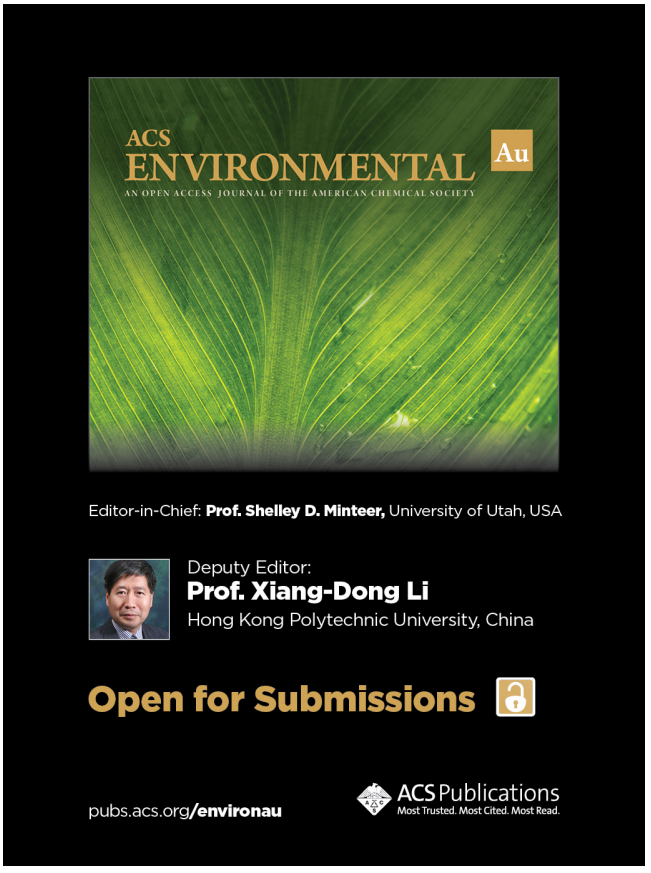
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