**Supporting Information**

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**A basic framework for calculating Total Annualized Cost (TAC) in a financial model.**
TAC is the sum of the Annualized Fixed Cost (AFC) and Operating Costs (OC). AFC is determined by dividing the Fixed Capital Investment (FCI) by the number of years, n, over which the costs are annualized. In this scenario, n is assumed to be 30 years. This model simplifies the cost analysis by focusing on annualizing fixed costs and adding them to the operating costs to understand the total yearly financial impact.

Annualized Fixed Cost (AFC) [1]: TAC= AFC + OC
TAC : Total Annualized Cost
AFC :Annualized Fixed Cost
OC : Operating Costs
For the time being, consider: AFC=FCI/n
In this study, we assume n=30 yr

**Table S1. Sugar production Cost in Different Level (feeding: sugar beet)[a]**

| Capacity level of a sugar plant | Lower limit of the range ($l_{s0}$) (mt $y^{-1}$) | Upper limit of the range ($l_{sl}$) (Mg $y^{-1}$) | Variable capital investment costs ($mt $y^{-1}$) | Fixed capital investment costs ($) |
|---|---|---|---|---|
| **Small ($l$ = 1)** | 800000 | 1400000 | 3.40 | 4258000 |
| **Medium ($l$ = 2)** | 1400000 | 3325000 | 2.72 | 6300000 |
| **Large ($l$ = 3)** | 3325000 | 4200000 | 2.34 | 11542600 |

[a] Optional: The study assesses the economic viability of sugar transformation into alternative commodities, accounting for domestic sugar demand. In the model, a factor of 0.23 can be applied to Equation 10, relating to capacity level ranges, to earmark 77% of sugar production for the domestic market. Equations S10 describe the modification:

$$(\zeta_l^{S,min} \times 0.23) \times e_{j,l}^S \leq s_{j,l}^S \leq (\zeta_l^{S,max} \times 0.23) \times e_{j,l}^S, \forall j \in J; \forall l \in L \quad [S10]$$

This reservation aligns with the assumption that selected sugar plants for the bio-technology supply would allocate a substantial portion of their output internally, thereby avoiding cost underestimation. Exclusively considering sugar for bioprocessing could lead to inaccuracies in representing sugar plant capacities. The factor (0.23) is derived from USDA(https://fas.usda.gov/data/commodities/sugar) and Statista data (https://www.statista.com/statistics/191975/sugarcane-production-in-the-us-by-state/), noting that of the 8.42 million tons of sugar produced between 2022 and 2023, approximately 2 million tons were exported, constituting roughly 23% of the total production, therefore 77% of sugar production for internal U.S. market.

**Table S2. IPA production Cost in Different Level**

| Capacity level of a sugar plant | Lower limit of the range ($l_{s0}$) (mt y–1) | Upper limit of the range ($l_{sl}$) (mt y–1) | Variable capital investment costs ($mt–1) | Fixed capital investment costs ($) |
|---|---|---|---|---|
| **Small ($l$ = 1)** | 6000 | 18000 | 28.06 | 360890.31 |
| **Medium ($l$ = 2)** | 18000 | 45000 | 18.94 | 697666.67[a] |
| **Large ($l$ = 3)** | 45000 | 90000 | 13.85 | 1208960.13 |

[a] AFC=FCI/n = 2.93M$/30 yr= 697666.67 $/yr

**Table S3. Transportation Cost of Sugar Beet and Sugar** [2]

| Symbol | Description | Unit | Value (estimate) |
|---|---|---|---|
| $t_{v1}$ | Variable transportation cost of sugar beets | $ Mg–1 km–1 | 0.25 |
| $t_{v2}$ | Variable transportation cost for sugar | $ Mg–1 km–1 | 0.09 |
| $t_{f1}$ | Fixed transportation cost (including loading and unloading) sugar beets | $ Mg–1 | 3.19 |
| $t_{f2}$ | Fixed transportation cost (including loading and unloading costs) for sugar | $ Mg–1 | 6.60 |

**Table S4. Ethanol Plant location in Minnesota, $CO_2$ Emissions, and Sugar Feed Support for IPA Plants**

| Ethanol Plant | Location | Annual Production (million gallons) | Million mt $CO_2$ emission | mt of sugar feeds in the IPA plant that can be supported by the CO2 emissions from ethanol plants [a] |
|---|---|---|---|---|
| 1 | Marshall | 50 | 0.13 | 95588.23 |
| 2 | Claremont | 130 | 0.338 | 248529.41 |
| 3 | Atwater | 90 | 0.234 | 172058.82 |
| 4 | Benson | 50 | 0.13 | 95588.23 |
| 5 | Morris | 30 | 0.078 | 57352.94 |
| 6 | Luverne | 21 | 0.0546 | 40147.06 |
| 7 | Granite Falls | 70 | 0.182 | 133823.53 |
| 8 | Fairmont | 119 | 0.3094 | 227500 |
| 9 | Fergus Falls | 60 | 0.156 | 114705.88 |
| 10 | Winnebago | 48 | 0.1248 | 91764.70 |
| 11 | Janesville | 165 | 0.429 | 315441.17 |
| 12 | Winthrop | 110 | 0.286 | 210294.12 |
| 13 | Heron Lake | 72 | 0.1872 | 137647.06 |
| 14 | Lamberton | 59.5 | 0.1547 | 113750 |
| 15 | Glenville | 45 | 0.117 | 86029.41 |
| 16 | Bingham Lake | 35 | 0.091 | 66911.76 |

| | | | | |
|---|---|---|---|---|
| 17 | Lake Crystal | 69 | 0.1794 | 131911.76 |
| 18 | Preston | 50 | 0.13 | 95588.23 |
| 19 | Welcome | 130 | 0.338 | 248529.41 |

[a] Determine the feasible scale of the IPA plant based on the available $CO_2$ emission from the ethanol plant.

**Table S5. Sugar Plant location in Minnesota**

| Company [a] | location |
|---|---|
| American Crystal Sugar | Crookston, MN |
| American Crystal Sugar | Moorhead, MN |
| American Crystal Sugar | East Grand Forks, MN |
| Minn-Dak Farmers Cooperative | 7525 Red River Rd W, Wahpeton, ND 58075 |
| Southern Minnesota Beet Sugar Cooperative | Renville, MN |

[a] In Minnesota, around 3,500 family-owned farms cultivate sugar beets, which are then processed by three farmer-owned cooperatives: American Crystal Sugar, Minn-Dak Farmers Cooperative, and Southern Minnesota Beet Sugar Cooperative. These cooperatives not only process the beets into sugar but are also entirely owned and operated by the farmers themselves.

**Table S6. 2018 Sugar Beet Supply by County in Minnesota: Annual Capacities and Costs.**

| Sugar beet supply county | Year | State | Ag District | County | Annual Capacity | Cost ($/mt) |
|---|---|---|---|---|---|---|
| 1 | 2018 | MINNESOTA | CENTRAL | KANDIYOHI | 326000.00 | 52.7 |
| 2 | 2018 | MINNESOTA | CENTRAL | MCLEOD | 29500.00 | 52.7 |
| 3 | 2018 | MINNESOTA | CENTRAL | MEEKER | 54500.00 | 52.7 |
| 4 | 2018 | MINNESOTA | CENTRAL | RENVILLE | 641000.00 | 52.7 |
| 5 | 2018 | MINNESOTA | CENTRAL | SIBLEY | 57700.00 | 52.7 |
| 6 | 2018 | MINNESOTA | CENTRAL | STEARNS | 92300.00 | 52.7 |
| 7 | 2018 | MINNESOTA | NORTHWEST | BECKER | 179000.00 | 50.6 |
| 8 | 2018 | MINNESOTA | NORTHWEST | CLAY | 1119000.00 | 50.6 |
| 9 | 2018 | MINNESOTA | NORTHWEST | KITTSON | 527000.00 | 50.6 |
| 10 | 2018 | MINNESOTA | NORTHWEST | MAHNOMEN | 64200.00 | 50.6 |
| 11 | 2018 | MINNESOTA | NORTHWEST | MARSHALL | 875000.00 | 50.6 |
| 12 | 2018 | MINNESOTA | NORTHWEST | NORMAN | 1140000.00 | 50.6 |
| 13 | 2018 | MINNESOTA | NORTHWEST | PENNINGTON | 27500.00 | 50.6 |
| 14 | 2018 | MINNESOTA | NORTHWEST | POLK | 2673000.00 | 50.6 |
| 15 | 2018 | MINNESOTA | NORTHWEST | RED LAKE | 29300.00 | 50.6 |
| 16 | 2018 | MINNESOTA | SOUTHWEST | REDWOOD | 76800.00 | 52.7 |
| 17 | 2018 | MINNESOTA | WEST CENTRAL | CHIPPEWA | 573000.00 | 52.7 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 18 | 2018 | MINNESOTA | WEST CENTRAL | GRANT | 239000.00 | 52.7 |
| 19 | 2018 | MINNESOTA | WEST CENTRAL | OTTER TAIL | 51400.00 | 52.7 |
| 20 | 2018 | MINNESOTA | WEST CENTRAL | POPE | 116000.00 | 52.7 |
| 21 | 2018 | MINNESOTA | WEST CENTRAL | STEVENS | 133000.00 | 52.7 |
| 22 | 2018 | MINNESOTA | WEST CENTRAL | SWIFT | 213000.00 | 52.7 |
| 23 | 2018 | MINNESOTA | WEST CENTRAL | TRAVERSE | 178000.00 | 52.7 |
| 24 | 2018 | MINNESOTA | WEST CENTRAL | WILKIN | 972000.00 | 52.7 |
| 25 | 2018 | MINNESOTA | WEST CENTRAL | YELLOW MEDICINE | 69400.00 | 52.7 |

**The $CO_2$ source assumptions for Minnesota's ethanol fermentation process can be summarized as follows:**

1. The state's total $CO_2$ emissions from this process are approximately 3.65 million metric tons per year [3].
2. These emissions are allocated based on the scale of each ethanol plant.
3. Ethanol production from corn and biomass generates a biogenic $CO_2$ stream that is 99.9% pure [4], requiring only the removal of excess water before compression and transportation.
4. There are no transportation costs for $CO_2$ as it is sourced directly from the ethanol plants, which also limits the capacity of IPA plants.
5. The $CO_2$ cost includes:
    a. Capital Expenditure (CapEx): Calculated as 0.15 times the plant size in million gallons per year plus 9 million dollars [3].
    b. Operating expenses for capture, compression, and dehydration are $8.58 per metric ton processed.

**Table S7. Global Warming Potential (GWP) of Various Agricultural and Industrial Activities: ReCiPe Midpoint (I) Assessment**

| Activity | unit | location | ReCiPe Midpoint (I) \| climate change \| GWP100 |
|---|---|---|---|
| sugar beet production | kilogram | US | 0.079 |
| beet sugar production | kilogram | RoW | 0.189 |
| ethanol production from sugar beet | kilogram | RoW | 0.097 |
| market for transport, tractor and trailer, agricultural | ton kilometer | RoW | 0.358 |
| DAC CO2 | kg | GLO | -0.880 |

| | | | |
|---|---|---|---|
| bio-IPA production process (small scale) | kg | GLO | 5.540 |
| bio-IPA production process (medium scale) | kg | GLO | 3.570 |
| bio-IPA production process (large scale) | kg | GLO | 2.470 |

**Technoeconomic Analysis (TEA):**

**TEA.1 - Flowsheet for the proposed mixotrophic isopropanol (IPA) production (benchmark case):**
We built a model for a simplified production process based on the proposed synthetic syntrophic consortia using Aspen Plus ®V12 simulation software to generate feasible flowsheet variants. Raw material and energy were used for TEA. 108,000 kg of glucose per cycle of fermentation (48 hours) is selected as the modeling plant size. IPA production and purification flowsheets encompass the bioreactor, the beer column for separating 99 wt.% of water and acids from the fermentation flows, and the distillation towers for purification purposes. The model includes the consideration of a separation unit for mixed alcohols and the investigation of extractant recycling. The products form two binary azeotrope systems (IPA/$H_2O$ and EtOH/$H_2O$); therefore, in the extractive distillation design, ethylene glycol serves as an effective extractant to break the azeotropes by increasing the relative volatility of the mixture of alcohols and water. The Glucose: $CO_2$ ratios of 1:3 case, achieved the purity of the alcohol 96 wt.%. The design input scale is 108,000 kg glucose/cycle (48 hours per cycle). The annual production is around 13,730 metric tons of isopropanol and 2622 mt of ethanol, with above 97 wt.% product recovery.

**TEA.2 - Sensitivity analysis:**
We applied discounted cash flow rate of return analysis to calculate the minimum selling price (MSP) of the alcohols which was derived when the net present value equaled zero. The reported MSP of the benchmark case is 710.28$/mt of IPA. Building upon the economic performance of the design, an in-depth sensitivity analysis was conducted to measure the effect of alterations in the cost of raw materials on the MSP and understand the correlation between plant capacity and MSP for the improved design. As derived from the cost assessment, the cost of raw materials is the predominant factor influencing the MSP. Geographic location and source substantially alter the cost of these raw materials. With a ±10% fluctuation in material (sugar) prices, the MSP (IPA) sees a deviation of +/-5.2%.

**TEA.3 - Comparing prices with current chemical technology:**
The current IPA US market price is reported at around 1560.0 $/mt (Echemi.com platform, a global chemical industry B2B website, accessed 2023-12-20). Based on the estimated MSP $CO_2$/Glucose=3 process with two purification designs are economically feasible and competitive (MSP for the model, 710.28$/mt). Moreover, the proposed synthesis pathway is compared with the current industrial approach (Isopropyl Alcohol**,** Logsdon, EJ & Locke, RA (2000); https://doi.org/ 10.1002/0471238961.0919151612150719.a01): an indirect hydration process with propylene as the primary raw material. With the use of same economic parameters, the MSP of the indirect hydration process is 988.67 $/mt. The TEA results suggest that the biological process is cost-competitive, and there is an expected 30% cost reduction of IPA compared to the conventional fossil fuel route. (FOB Texas price of IPA oscillated between $1310-1320).

**TEA.4 - Additional Techno-economic Analysis Assumptions of the bio-IPA process:**

1) All equipment and operating costs were estimated in Aspen Process Economic Analyzer V12 with 2014 as the cost basis, and bioreactors were determined using the prices provided by Matches (2014) [5].

2) The project's economic life was set at 20 years with a 10-year recovery period. The internal rate of return targeted was 10% with a 21% corporate tax applied to profits. Depreciation was calculated using the straight-line method and a 5% salvage value was assumed after 20 years. To determine the minimum selling price (MSP), a discounted cash flow analysis was performed, which calculates the product's selling price when the net present value (NPV) equals zero.

3) The market price of glucose is $ 0.15/lb [6]; ethanol by-product selling price is 960 $/mt

4) Ethylene glycol (EG) is used as the extractant, believed to preserve properties, and prevent decay. EG is bought at $484/ mt .

5) The cost of water for the fermentation process is assumed to be $100/t. It is assumed that carbon dioxide gas could be taken as free, for the tradeable existing $CO_2$ federal tax credits (carbon tax rate is $54 per metric ton ($2023))[8].

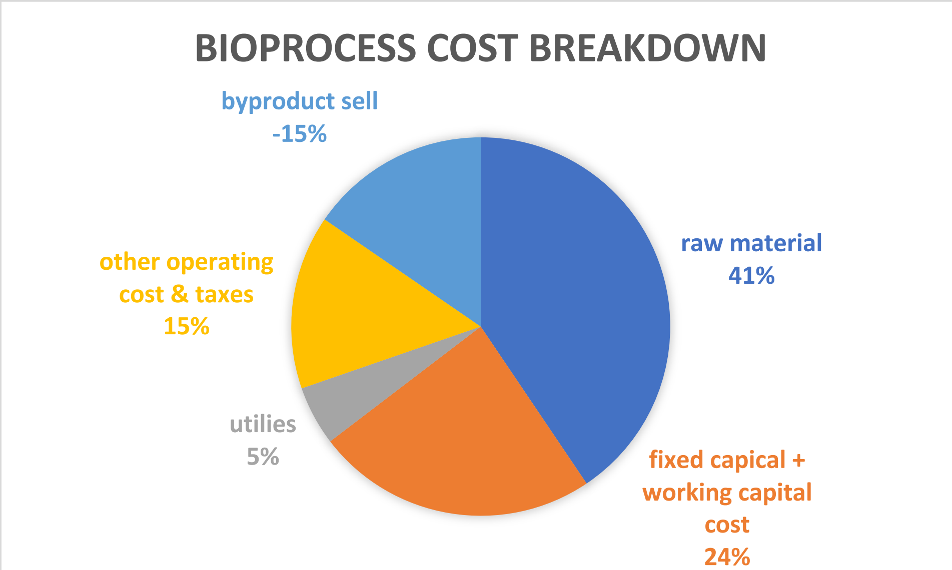
6) For the estimation of operating cost in the bio-process that use in the supply chain model, the byproduct selling price is contribute to the unit operating cost

**Table S8. Annual capital and operating cost.**

| Item | Cost (Million $) | Item | Cost per year (Million $) |
|---|---|---|---|
| Purchased Equipment | 6.00 | Total Raw Materials Cost | 6.55 |
| Other | 11.21 | Total Utilities Cost | 0.82 |
| General and Administrative Overheads | 0.48 | Operating Labor Cost | 0.92 |
| Contract Fee | 0.52 | Maintenance Cost | 0.20 |
| Contingencies | 1.72 | Operating Charges | 0.20 |
| Working Capital | 1.00 | Plant Overhead | 0.58 |
| Total Capital Cost | **20.93** | General and Administrative Cost | 0.45 |
| Sell of by-product (EtOH)[a] | **2.49** | Total Operating Cost | **3.17** |

[a] The revenue from by-product sales ($) is observed to rise linearly with the raw material (sugar, the substrate) costs. The Operating Cost (OC) parameters used in the supply chain model was computed as the total operating expenses minus the raw material costs, adjusted by the revenue from by-product sales. The premise for this assumption is the preliminary site selection for the supply chain, positing that the IPA biorefinery will be sited adjacent to an established ethanol facility in Minnesota. The by-product ethanol is sent to the ethanol plant for sell.

**Figure S1. Cost breakdown of the IPA bio-process.**




**TEA.5 - Additional Techno-economic Analysis Assumptions of the IPA production process via**

The proposed bio-synthesis pathway is compared with the current industrial approach [9]: an indirect hydration process with propylene as the primary raw material. The TEA results suggest that the biological process is cost-competitive

1) Assumptions for Indirect Hydration Process: Reaction Pathways: Indirect hydration using a 60% acid solution at 75-85°C and 0.6-1 MPa. Note: Strong-acid process is not commercially important due to high-purity propylene feed requirements and similar disposal issues

2) Hydrogen Usage: Fermentation off-gas (from *Cac*) contributes to meeting some $CO_2$ fixation hydrogen demands [10]. Additional hydrogen assumed to be free based on DOE's hydrogen hubs projects and aligned with US Department of Energy ARPA-E program funding [10]. This funding aims to accelerate the commercial-scale deployment of low-cost, clean hydrogen as an alternative source of energy and to create networks of clean hydrogen producers, consumers, and infrastructure. The DOE has selected seven potential $H_2$ hub locations for further negotiation, including the Heartland Hydrogen Hub (Minnesota, North Dakota, South Dakota) [11]. Up to $925 million will be available to leverage the region's abundant energy resources to help decarbonize the agricultural sector's production of fertilizer, decrease the regional cost of clean hydrogen, and use clean hydrogen for power generation.

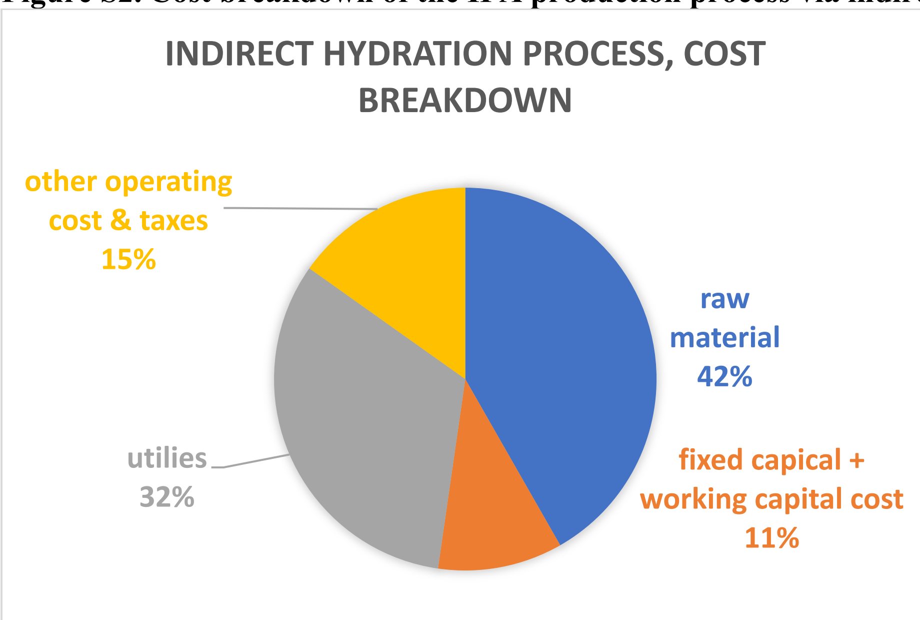
3) Minimum Selling Price Calculation of isopropanol: $1649.1 per metric ton

4) Feedstock and Market Prices: Propene price is $0.584/kg.

| Item | Cost (Million $) | Item | Cost per year (Million $) |
|---|---|---|---|
| Purchased Equipment | 102.24 | Total Catalyst Cost | 0.00 |
| Other | 7.11 | Total Raw Materials Cost | 16.77 |

| | | | |
|---|---|---|---|
| General and Administrative Overheads | 3.06 | Total Utilities Cost | 13.09 |
| Contract Fee | 3.28 | Operating Labor Cost | 0.90 |
| Contingencies | 10.94 | Maintenance Cost | 0.10 |
| Working Capital | 6.33 | Operating Charges | 0.23 |
| Total Capital Cost | **25.35** | Plant Overhead | 0.50 |
| | | General and Administrative Cost | 2.75 |
| | | Total Operating Cost | **34.32** |

**Figure S2. Cost breakdown of the IPA production process via indirect hydration.**




**Reference**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