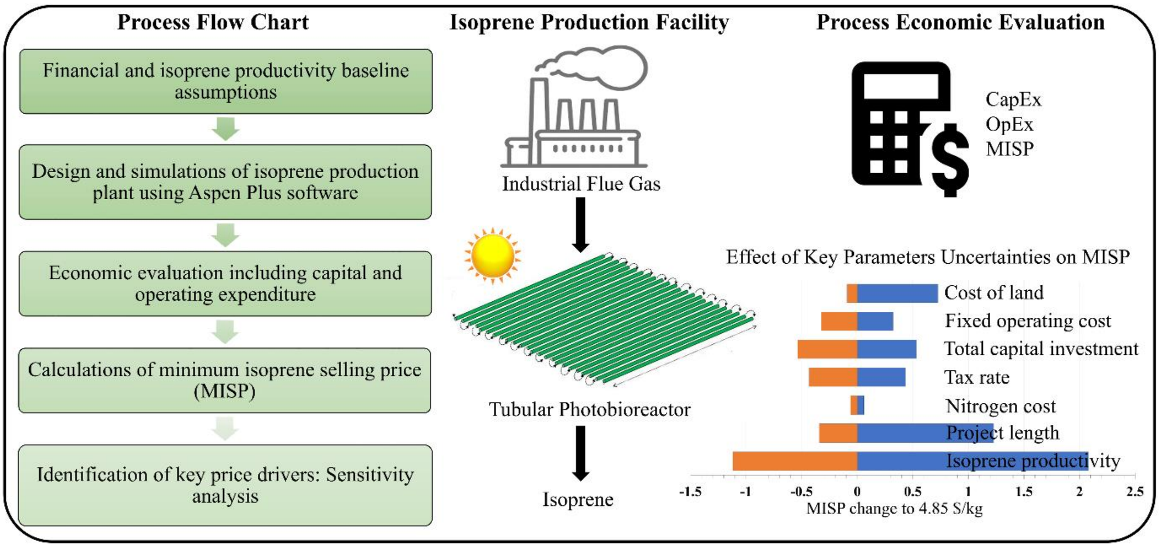
Chapter – 5

Design and simulation of isoprene production plant using flue gas as sole carbon source and its techno-economic analysis



Indrajeet Yadav et al. (2023) Carbon dioxide sequestration and transformation into isoprene using engineered cyanobacteria *Synechococcus elongatus* UTEX 2973 and its techno-economic assessment. Journal of cleaner production (***communicated***)

5.1 Background

Growing concerns surrounding climate change, energy security, and rural development have sparked a focus on renewal biofuels, particularly biofuels for transportation (Beal et al., 2015). Biomass sequesters carbon dioxide from the atmosphere, making effective conversion and utilization for biofuels a potential avenue for reducing reliance on fossil fuels and ultimately lowering net carbon dioxide (CO_2) emissions (Yadav et al., 2019). In recent years, there has been significant exploration of sustainable biofuel production technologies, given their essential role in advancing a green and circular biobased economy. While the current lab-scale experimental results are promising, it is crucial to conduct a comprehensive analysis and evaluation of the economic viability and practical applications on an industrial scale. This study proposes the implementation of a comprehensive techno-economic analysis (TEA), which provides a structured framework for quantitatively assessing the economic performance of a particular process design. This evaluation is based on existing research in bioconversion and process integration, considering factors such as cost, benefits, risks, sensitivity and uncertainties (Liang et al., 2022; Markham et al., 2016; Zhang et al., 2018). The objective is to device its potential for future commercialization and provide guidance for research and investment in the most advantageous direction. The objective of this TEA study is to assess the economic viability of proposed scenario for converting flue gas (CO_2) into isoprene using photosynthetic engineered cyanobacterial production system. This evaluation involves comparisons of capital costs, operating costs, and the minimum isoprene selling price (MISP). Additionally, sensitivity analysis was conducted to provide direction for the engineering aspects of isoprene production with the highest economic potential. The findings from this study will assist researchers and decision-makers in prioritizing key economic drivers to enhance the techno-economic efficiency of CO_2 bioconversion for isoprene production.

5.2 Materials and methods

A conceptual large-scale isoprene production plant was designed in which recombinant cyanobacteria (*S. elongatus* UTEX IspS.IDI) is proposed to be used for photosynthetic production of isoprene using industrial flue gas as CO_2 source. The model of plant was designed and simulated for material and energy balances using Aspen Plus software (AspenTech, Cambridge, MA, USA). Preliminary economic evaluation including total capital expenditure (CapEx) and annual operating expenditure (OpEx) were investigated using Aspen Process Economic Analyzer. Furthermore, MISP was determined using a discounted cash flow method (10-year) with zero net present value (NPV) and internal rate of return (IRR) 10%. Sensitivity analysis was performed on seven critical performance metrics to identify variables having the greatest impact on the isoprene production process so that technologists can optimize the process to be more efficient and cost-effective.

5.2.1 Assumptions and process description

A schematic process flow diagram of large-scale isoprene production plant has been presented in Figure 5.1. For achieving an annual isoprene production of 1000 tonne, a conceptual design of photobioreactor (PBR) of 100 m^3 (working volume) continuous production system was proposed based on the preliminary data obtained from lab scale experimental results and literatures. The Inside Battery Limit (ISBL) of isoprene manufacturing facility comprises five main operational units: gas supply, isoprene production, isoprene recovery, biomass separation and wastewater treatment and recycle units. The assumptions presented in Table 5.1 were derived from a comprehensive review of the literature.

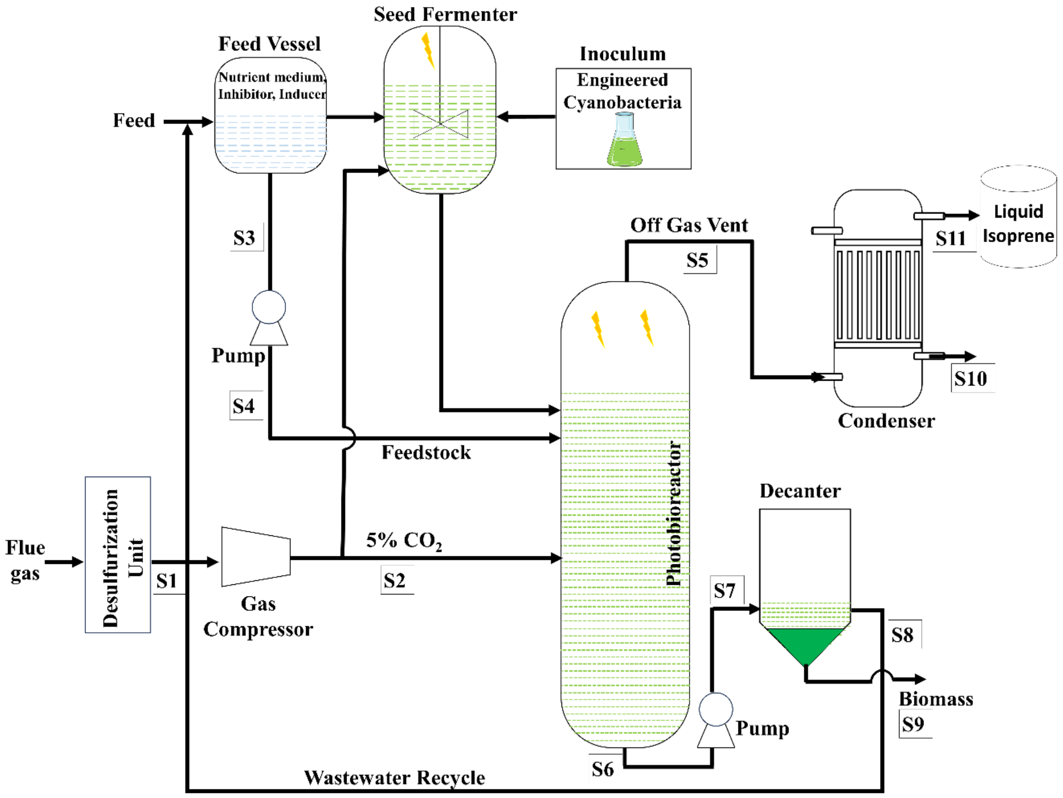


Figure 5.1 Simplified process flow diagram of cyanobacterial isoprene production plant. (S1) Purified flue gas compressor stream, (S2) Purified flue gas photobioreactor stream, (S3) Nutrient feed pump stream, (S4) Nutrient feed photobioreactor stream, (S5) Off gas vent condenser stream, (S6) Cyanobacterial culture pump stream, (S7) Cyanobacterial culture decanter stream, (S8) Wastewater stream, (S9) Biomass stream, (S10) O_2 stream, (S11) Isoprene stream.

5.2.2 Gas supply unit

The proposed CO_2 source for the isoprene production plant will be industrial flue gas delivered through a dedicated pipeline from a power plant located directly nearby the facility. Previous works have demonstrated the feasibility of using flue gas, containing 3-6% (v/v) CO_2, as the exclusive carbon source for squalene synthesis using engineered *Synechococcus elongatus* 7942 (Choi et al., 2020). In current work, flue gas, serving as the sole carbon source, was supposed to channelled directly from the power plant to the cultivation site via pipelines.

Table 5.1 Financial and productivity baseline assumptions for techno-economic analysis of isoprene production plant.

Financial assumption	**Value**
Internal rate of return	10%
Plant financing by equity	50%
Plant life (years)	20
Income tax rate	20%
Interest rate of debt financing	8%
Term for debt financing (years)	10
Depreciation schedule (years)	7
Startup time (years)	0.5
Productivity baseline assumptions	
Production scale (tonnes/year)	1000
Facility size (acres, PBRs only)	604
Total facility size (acres)	719
PBR volume (m^3)	100
Total number of PBRs used	407
Isoprene productivity ($g/m^3/day$)	74.4
Batch time (day)	60
Down time (day)	6
Operating days per year	330

This gas mixture contains 3-6% (v/v) CO_2, 11.99% (v/v) O_2, 21.72 ppm NOx, 1.43 ppm CO, water vapor, and dust (Choi et al., 2017). The Sulfur was eliminated through the desulfurization process using a flue gas desulfurization system (FGD) as previously demonstrated by Choi et al. (2020). Following desulfurization, the flue gas was introduced into the PBRs through direct injection at a flow rate of 0.1 VVM. The flue gas was subjected to compression up to 5 bar using a gas compressor in order to stabilize the pressure and meet the required fermentation conditions in PBRs (Liang et al., 2022). It is assumed that these photobioreactors assimilate approximately 90% of the CO_2, distributed between isoprene production and biomass formation in a ratio of 80:20 while remaining 10% being contained in PBR headspace (Markham et al., 2016). To achieve an annual production capacity of 1000 tonnes of isoprene, the necessary amount of flue gas was calculated considering 5% CO_2 content. While there is no additional operating cost for utilizing CO_2 from flue gases, a slight upfront capital expenditure is required for FGD installation. Based on established CO_2 allowance initiatives, zero cost or even income is expected on flue gas utilization (Llamas et al., 2021). However, flue gas management and handling may impact the overall cost of the production facility. The European Union introduced a carbon emissions reduction mechanism through an emissions trading system for greenhouse gases, enabling the trading of emission rights when anthropogenic CO_2 is employed in production facilities. The system has the capacity to capture anthropogenic CO_2 emissions, treating it as revenue in the form of CO_2 allowance (Llamas et al., 2021).

5.2.3 Isoprene production unit

The Aspen Plus software was employed to simulate the process of isoprene production in tubular PBRs (80% working volume) having working volume of 100 m^3. This simulation considered two primary reactions taking place within the PBRs, biomass and isoprene synthesis as described by Equation 5.1 and Equation 5.2, respectively.

$$CO_2 + 0.622H_2O + 0.23NH_3 = CH_{1.939}O_{0.473}N_{0.23} + 1.0745O_2 \qquad (5.1)$$

$$5CO_2 + 4H_2O = C_5H_8 + 7O_2 \qquad (5.2)$$

The stoichiometric equations for generating biomass by cyanobacteria (Equation 5.1) used in Aspen simulations was derived from previously published literatures (Liang et al., 2022). The empirical formulas $CH_{1.934}O_{0.473}N_{0.23}$ represents the biomass produced by cyanobacteria. There are various designs available in the literature for photosynthetic bioreactors used in algae and cyanobacteria cultivation for production of bioproducts and biofuels. Given that isoprene is a highly volatile compound, it evaporates under standard production conditions. This imposes the use of a closed system for collecting isoprene from the gas phase of the photosynthetic PBRs. A system consisting of rigid tubular PBRs is chosen as the base case design. These PBRs are composed of a series of parallel tubes with an inner diameter of 8 cm and sections that are 80 meters long, as specified earlier (Davis et al., 2011; Markham et al., 2016). The area of total land required is calculated as described in previous studies that PBR tubes having volume of 200 m^3 covers 1 hectare land (Davis et al., 2011; Markham et al., 2016). The PBRs utilizes airlift column degassing stations to eliminate the gas phase. The gas mixture from the headspace is send to an isoprene recovery unit for the capture and purification of isoprene. The residual CO_2 is then recycled back into the PBRs. These reactors are assumed to function as closed systems, with no losses due to evaporation. Using this type of setup could provide a constant productivity of isoprene, despite the individual reactors having different rates of isoprene production due to variation in cyanobacterial growth phase, light irradiance, nutrient availability, and other growth conditions. The design parameters are configured to generate 1000 tonnes of isoprene annually. The cultivation systems are anticipated to operate continuously, with the off-gases being constantly transferred to isoprene recovery unit. It is assumed that the culture in each closed PBRs will be refreshed every 60 days (turnover time), and the cyanobacterial biomass will be harvested in biomass recovery unit (Markham et al., 2016).

The wastewater will be directed to wastewater treatment area and the treated water is subsequently recycled to the PBRs.

5.2.4 Isoprene recovery

In commercial production, technologies for purifying isoprene from light olefins a range of methods exists, including cryogenic separation, selective binding onto nonpolar surfaces and gas stripping with solvent recovery. In this study a cryogenic separation using a condenser was considered. Due to high volatility of isoprene, it readily exits the photobioreactor as part of the off-gas during the fermentation process. The gas phase from the cultivation systems, which includes isoprene, residual CO_2, water vapor and oxygen is then sent to the isoprene recovery unit through an amine-based solution. Due to the tendency of CO_2 to solidify under cryogenic conditions, a pre-treatment step involving amine-based residual CO_2 capture is employed in the cryogenic separation process. This ensures efficient downstream isoprene separation by preventing CO_2 solidification-related problems (Markham et al., 2016). Furthermore, the gas mixture undergoes water vapor removal via targeted adsorption onto molecular sieves. This dehydration step is crucial for efficient downstream isoprene condensation and process integrity. Lastly the isoprene gets condensed in to the condenser at very low temperature and separated as previously demonstrated by Matos et al. (2013). The isoprene-rich gas mixture undergoes final isolation within the condenser. Utilizing cryogenic temperatures, the isoprene condenses from the gas phase, facilitating its physical separation from the remaining components.

5.2.5 Biomass recovery

The plant utilizes a decanter to achieve optimal separation of the biomass from the post-fermentation broth. The biomass recovery unit enables the recovery and transformation of cyanobacterial biomass into diverse value-added bioproducts. While achieving complete conversion of cyanobacterial biomass into biofuels and chemicals through a self-sustained biorefinery system poses challenges, it offers the potential for producing a range of valuable products such as lipids, carotenoids, proteins, nutraceuticals, carbohydrates, and feedstocks through the valorization of biomass. The resulting wastewater is subjected to additional treatment in the wastewater treatment unit before being recycled for use in the PBRs.

5.2.6 Economic evaluations

Completion of the simulation provided a platform for extracting mass balances from the process, enabling a comprehensive assessment of production costs and a meaningful return period estimation. The estimated operational costs for the proposed plant are derived from material and energy balance analyses conducted using Aspen Plus process simulations. The raw material unit costs are estimated according to literature or existing models and summarized in Table 5.2. The primary raw materials used in the process include flue gas, diammonium phosphate, ammonia, IPTG, alendronate, water and electricity. The produced biomass can be utilized as a biofertilizer or valorized to yield high-value bioproducts, such as carotenoids, proteins, and lipids, which can be commercialized as secondary products. Equipment sizing and capital expense calculations are determined based on material, energy balance, and flow rate data using Aspen Process Economic Analyzer.

Table 5.2 Cost of raw materials used in the base case isoprene production study.

Materials	Cost	Unit	Source
Ammonia	431	\$/ tonne	Liang et al. (2022)
K_2HPO_4	724.35	\$/ tonne	Markham et al. (2016)
Water	0.2	\$/ tonne	Liang et al. (2022)
Inducer (IPTG)	7000	\$/ tonne	Vendor quotation
Inhibitor (alendronate)	1000	\$/ tonne	Vendor quotation
Electricity	0.1	\$/KW	Liang et al. (2022)

Equipment cost sources include vendor quotations, prior published research projects, national renewable energy laboratory (NREL) design reports, and internal equipment costing databases. For example, cost of PBRs is drawn from a previous study reported by Liang et al. (2022). The costs of certain standardized process equipment, such as condensation columns, pumps, and tanks, are derived from estimations made using software Aspen Process Economic Analyzer. The capital expenditures were estimated by considering the overall expenses associated with the purchase and installation of equipment. To estimate equipment costs for varied production scales, an exponential scaling equation was utilized (Equation 5.3).

$$(\text{New cost} = \text{Base cost} \times (\text{New size}/\text{Base size})^{n} \qquad (5.3)$$

Where n is the economy scaling factor that varies with the equipment based on the equipment size specified in the original price quote.

The total operating expenses (OpEx), comprising variable operating cost (VOC) and fixed operating costs (FOC) were obtained from available TEA reports have been adjusted to reflect 2023-dollar values. For the DCF analysis, 40% equity financing at 8% interest over 10 years forms the financial baseline. A straight-line depreciation method is utilized for the plant, with a seven-year depreciation period. The MISP is the price at which the isoprene, must be sold to achieve an IRR of 10% and an NPV of zero at year 20. The base case model employs PBRs for isoprene production coupled with cryogenic separation. To comprehensively assess the model's robustness and identify potential optimization opportunities, sensitivity cases were developed exploring variations in key parameters and alternative approaches to cultivation.

5.3 Results and discussions

5.3.1 Base case process description

In our previous reported study, *IspS* and *IDI* genes were inserted at NSI and NSIII sites respectively into the genomic DNA of *S. elongatus* UTEX 2973 which resulted recombinant strain *S. elongatus* UTEX IspS.IDI (Yadav et al., 2023a). Moreover, to enhance the isoprene production, an inhibitor (alendronate) was employed for blocking the terpenoid synthetic pathway by inhibiting CrtE enzyme. The engineered cyanobacterial strain *S. elongatus* UTEX IspS.IDI was able to produce isoprene with an average productivity of 31 µg/L/h (0.744 g/m^3/day) in the presence of alendronate (20 µg/mL) and IPTG (1 mM) in sealed serum bottles in batch mode at optimized process conditions (Yadav et al., 2023b). As reported in previous studies, the accumulation of isoprene and oxygen in the headspace of culture vessel exerts the negative effect of isoprene productivity reducing the real productivity by 100-fold or more (Pade et al., 2016; Rana et al., 2022; Yadav et al., 2023b). Therefore, it was assumed that the productivity could be increased up to 100 times more reaching upto 74.4 g/m^3/day when isoprene production will be carried out in continuous mode in which the generated isoprene and oxygen will be removed continuously from the headspace of PBR. In the current isoprene production facility design, it is assumed that produced isoprene and other gases including unconverted CO_2 and oxygen would be transferred to isoprene recovery unit continuously passing through an amine solution to absorb the residual CO_2. The isoprene production facility comprising of tubular PBRs may achieve an isoprene productivity of 74.4 g/m^3/day in which industrial flue gas as sole source of CO_2 would be supplied to reduce the production cost. This target productivity serves as a key research milestone, suggesting a significant step forward beyond existing theoretical boundaries. It is crucial to acknowledge that this early-stage profitable technology has yet to be implemented at a larger scale. Hence, a conceptual precommercial analysis has been presented here, outlining potential estimates for technology scaling up in a proposed production plant. In a reported study, the isoprene recovery was performed by gas stripping using heptane as solvent and maintained its temperature – 40 °C using a cooling bath prepared by acetonitrile and dry ice (Rana et al., 2022). Cryogenic distillation is a well-established technology for isoprene purification in commercial applications, but it may potentially entail higher costs due to the substantial energy requirements for refrigeration of gas streams. Therefore, installation of a condenser has been proposed in isoprene recovery unit for isoprene separation and purification in an economic manner as previously demonstrated by Matos et al. (2013).

5.3.1 Capital cost expenditure (CapEx)

The equipment costs are estimated based on data from previous TEAs, published literature, vendor quotes, and Aspen Process Economic Evaluation software (Kumar et al., 2020; Liang et al., 2022; Markham et al., 2016; Oostlander et al., 2020; Pandey et al., 2020; Wiesberg et al., 2017). The percentage contribution of capital cost has been presented in in Figure 5.2A. The total installed equipment cost is estimated to be 5.705 million $, and the total capital investment is estimated to be 21.16 million $ (Table 5.3). As it is evident by literatures that photosynthetic production of biomolecules costs maximum on the production unit which includes PBRs and land (Mhatre et al., 2018; Pires et al., 2012; Price et al., 2022). In current study, the isoprene production unit, specifically the tubular PBRs, constitutes the major percentage among installed equipment cost, amounting to 2.822 million $. The collective cost of the PBRs, isoprene purification, and biomass separation units accounts for approximately 80% of the total equipment installed cost. Other capital expenses include contingencies, civil work, overheads, contracts, and design and engineering and constructions. The construction part is consisting of piping, civil, steel, instrumentation, electrical, insulation and paint which contributes total 13% of total capital expenditure.

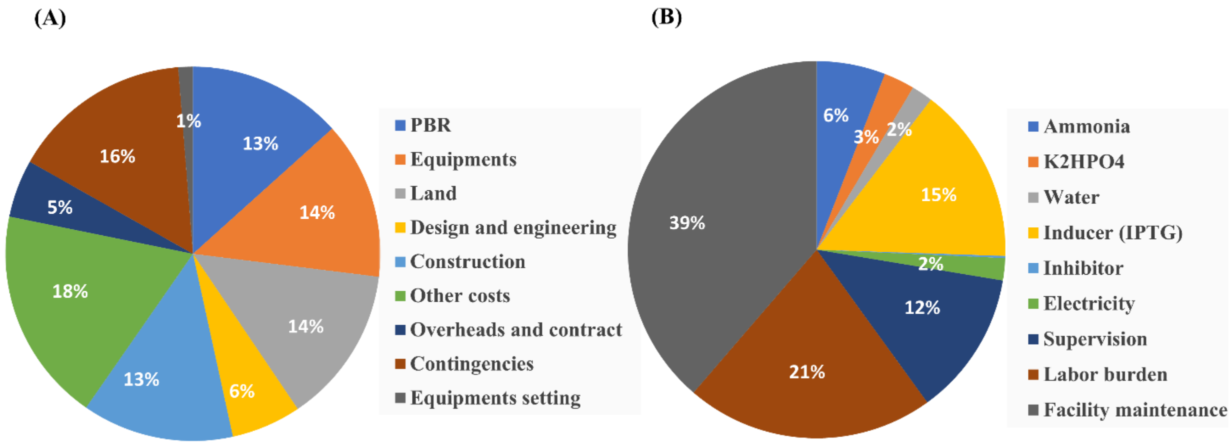


Figure 5.2 Cost breakdown of the isoprene production plant. (A) Capital cost contains the installed cost of operational units and other major expenses. (B) Annual operating expenses including both fixed (supervision, labor burden and maintenance) and variable costs (chemicals and electricity)

5.3.3 Operating expenditure (OpEx)

The operational expenses for the facility have been presented in Table 5.4. The operational costs were categorised into two categories i.e., VOC and FOC. The VOC includes the expenses covered by purchasing ammonia, inducer, inhibitor, makeup water/water disposal, purchased electricity, and other nutrients for cyanobacterial cell growth and maintenance. FOC covers all the expenditures that are used for manpower salaries, facility maintenance, and insurance and taxes. CO_2 is supplied in the form of flue gases assuming it's cost negligible. The component wise percentage distribution of operating costs has been presented in Figure 5.2B. The facility's largest operating expenses are supervision, labor burden and facility maintenance accounting total 1.617 million $/year. The second-highest operating expense is 0.339 million $ which is expensed on purchasing IPTG annually for isoprene production.

Table 5.3 Total project capital expenditure (CapEx) with costs of individual equipment and other costs associated with isoprene production plant.

Equipment	**Installed cost (million $)**[a]
Flue gas desulfurization unit	0.006
Gas compressor	1.073
Pumps	0.072
Closed tubular PBRs	2.822
Flash tank	0.161
Centrifuge	1.520
Condenser	0.052
Total equipment cost	5.705
Other costs	
Equipment Setting	0.266
Land	2.876
Piping	0.342
Civil	0.201
Steel	0.098
Instrumentation	0.844
Electrical	1.071
Insulation	0.184
Paint	0.029
Other	3.923
G and A Overheads	0.479
Contract Fee	0.577
Total Design, Eng, Procurement Cost	1.274
Contingencies	3.291
Total cost	15.455
Total Project Cost (equipment cost+ other costs)	21.16

[a] Equipment and other costs are based on the liang et al. (2022); Davis et al. (2011); Markham et al. (2016), and Aspen Process Economic Analyzer.

To reduce the purchase cost of CO_2, it was assumed that CO_2 has been obtained from a thermal power plant and delivered after preliminary treatment. Previous studies have been successfully utilised the industrial flue gases as sole carbon source after preliminary treatment to reduce the production cost of the molecule of interest (Pekkoh et al., 2023; Pires et al., 2012; Wang et al., 2023; Zieliński et al., 2023).

Table 5.4 Annual operating expenditure (OpEx) including fixed operating costs (FOC) and variable operating costs (VOC) for a plant of 1000-tonne isoprene production capacity.

Variable operating cost (Raw material)	**Annual cost (million $/year)**
Ammonia	0.132
K_2HPO_4	0.059
Water	0.041
Inducer (IPTG)	0.339
Inhibitor (alendronate)	0.004
Electricity	0.043
Sum of variable operating cost (VOC)	0.617
Fixed operating cost (FOC)	
Salaries	0.277
Labor burden	0.475
Facility maintenance	0.864
Sum of FOC	1.617
Total operating cost (VOC + FOC)	2.234

5.3.4 Minimum isoprene selling price

Setting a minimum selling price based on investment costs involves assessing the real-time expenses associated with a business decision (Liang et al., 2022; Markham et al., 2016). Based on the capital costs, production costs, and financial assumptions described in earlier sections, the MISP was calculated for base case and along with a range (upper and lower bound) of isoprene productivity levels. Based on a facility design of 1000 tonnes per year of isoprene production capacity, the resulting MISP is 4.85 $/kg considering a 10% IRR at base case isoprene productivity 74.4g/m^3/day. Figure 5.3 shows a negative correlation between MISP and isoprene productivity. An inverse relationship between product output and minimum selling price has been reported in prior studies. These findings demonstrate a decrease in minimum selling price with increasing the productivity, and vice versa. (Price et al., 2022; Sun et al., 2020). In this investigation, the MISP decreases with increasing productivity, ultimately reaching 2.42 \$/kg at a productivity of 148.8 g/m^3/day. Although the calculated MISP is 4.85 \$/kg for base case productivity, the actual market price of chemical grade isoprene is ranges between 5-50 \$/kg which suggests that photosynthetic isoprene production using engineered cyanobacteria from flue gases is an economically viable process. Based on current technology, CO_2-derived isoprene or other bioproducts is projected to be the most promising, assuming that CO_2 can be utilized with 90% efficiency (Davis et al., 2011; Markham et al., 2016). This TEA framework extends its application beyond the initial design and screening of conceptual process alternatives. It can be adapted and employed for similar bio-based production systems, providing valuable insights into research priorities and assisting in the establishment of criteria for successful technology implementation.

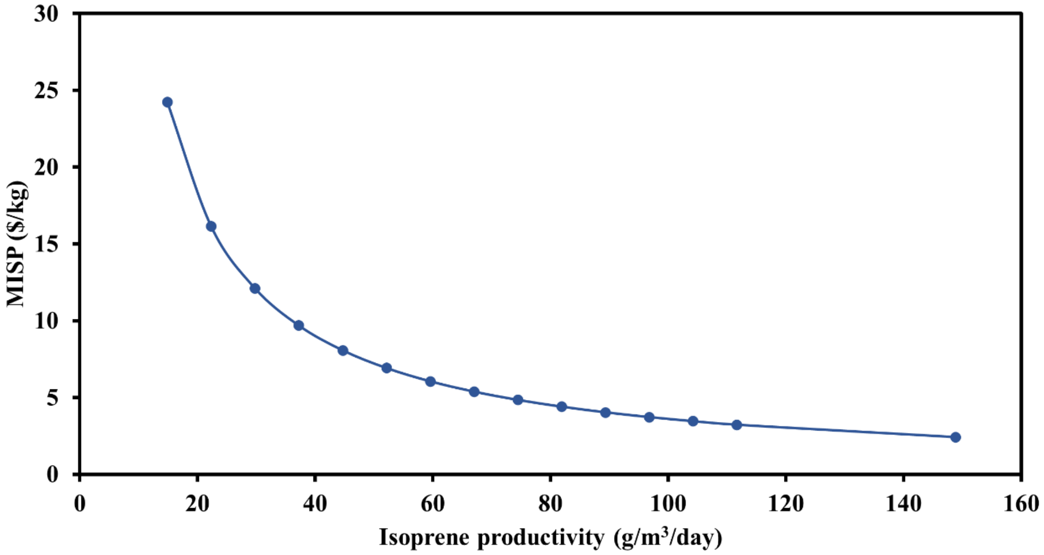


Figure 5.3 Effect of isoprene productivity on minimum isoprene selling price (MISP).

5.3.5 Sensitivity analysis

Sensitivity analysis was conducted to investigate how key variables affect the MISP and to identify variables to optimize the process economics. It is an effective way to measure the influence of key variables on the MISP (Regis et al., 2023; Tao et al., 2017). Therefore, a single-point sensitivity analysis was conducted on the CO_2-based isoprene production facility by changing one variable at a time between its lower and upper values, while keeping all other variables constant as performed in previous studies (Liang et al., 2022; Zhang et al., 2018). This research employs a targeted approach, investigating the influence of seven critical parameters related to photosynthetic isoprene production process on MISP. A baseline scenario was established with an isoprene productivity of 74.4 $g/m^3/day$ and a corresponding MISP of 4.85 $/kg. The baseline for all other variables was the same as the assumptions used in the base case. The study identified four key cost drivers for isoprene production: isoprene productivity, project length, cost of land and total capital investment. These factors, as shown in Figure 5.4, have a substantial impact on MISP with variations. Isoprene productivity and project length stand out as strong determinants of MISP, with a negative correlation with MISP which are similar to other reported studies (Liang et al., 2022; Markham et al., 2016). This implies that optimization of these factors is crucial for minimizing production costs. Doubling isoprene productivity from the base case dramatically reduces MISP by 50%, from 4.85 $/kg to 2.42 $/kg. Conversely, halving productivity leads to a significant increase of 100%, pushing MISP to 9.70 $/kg (Figure 5.4).

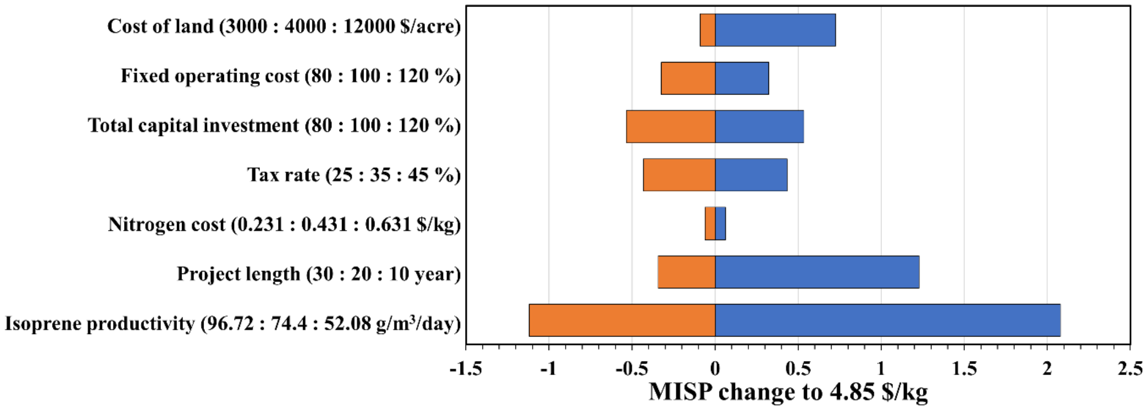


Figure 5.4 Impact of single point variations in parameters on the minimum isoprene selling price (MISP) (MISP is 4.85 $/kg in base case scenario) for the isoprene production process from flue gas.

Controlling light intensity and temperature in a large-scale isoprene production plant presents several significant challenges. Ensuring uniform light distribution across large bioreactor surfaces is difficult, leading to inconsistent growth conditions for the microbial culture. Additionally, maintaining optimal light intensity at such a scale requires significant energy, making it challenging to balance energy consumption with production efficiency. Temperature control poses another major issue, as large-scale systems are more susceptible to fluctuations, which can negatively impact microbial performance and isoprene productivity. Managing the heat generated during production also demands advanced cooling systems to maintain stable conditions. Moreover, neither light intensity nor temperature can be maintained at the desired (pre-determined) values in larger reactors as easily as in smaller 140 mL lab flasks. This inconsistency raises concerns about the equipment design and scaling used for economic analysis, potentially calling into question the accuracy and outcome of the entire economic feasibility study. External environmental factors, such as seasonal temperature variations and day-night light cycles, further complicate efforts to maintain consistent conditions, affecting production efficiency and overall feasibility (Markham et al., 2016).

5.4 Conclusion

A techno-economic analysis was conducted for a simulated plant of isoprene production aiming to produce isoprene using engineered cyanobacteria from CO_2 and light through continuous photo-fermentation. The design of an isoprene production process employing a 100 m^3 PBR and a base case productivity of 74.4 $g/m^3/day$ served as the starting point for further development. Cryogenic separation was selected as the preferred method for purifying isoprene from the PBRs headspace gas. Findings of this study strongly suggest that photosynthetic isoprene production is not only environmentally beneficial but also economically feasible. The estimated minimum selling price of 4.85 $/kg matches the MISP of existing microbial systems, paving the way for a potential shift towards more sustainable isoprene production. Furthermore, the sensitivity analysis determines key factors influencing the costs of the process, such as isoprene productivity, capital cost, project duration, and land cost. The most crucial factor for reducing costs was determined to be the productivity of isoprene. Enhancing the key factors in a collaborative manner is essential for achieving a more economically viable process. This study provides a platform for designing and cost optimization strategies for sustainable isoprene and other platform chemicals production utilizing flue gases.