

Article

Design and Techno-Economic Feasibility of a Sustainable Styrene Production Plant Integrating Corn Stover-Derived Bioethanol

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Abstract

This paper presents a comprehensive design, implementation, and feasibility analysis of a sustainable styrene production plant that integrates conventional ethylbenzene dehydrogenation with bio-based feedstock processing. Located on the Gujarat coastline, India, the proposed facility is designed to produce 220,000 tonnes per year of styrene while addressing environmental, social, and economic sustainability objectives. Agricultural corn stover sourced from local farms is valorised via pretreatment, enzymatic hydrolysis, and two-phase simultaneous saccharification and fermentation (TPSSF), achieving ethanol yields of up to 477 kg per tonne of biomass. Bioethanol is subsequently alkylated with benzene over a beta-zeolite catalyst, delivering a 95% conversion with respect to bioethanol and 85.8% selectivity to ethylbenzene. This intermediate is then dehydrogenated at 550 °C using a potassium-promoted iron oxide catalyst to produce styrene with a 96.2% selectivity. Extensive heat integration, benzene recycling, and a steam-to-ethylbenzene ratio of 7:1 enhance energy efficiency and process robustness. Techno-economic analysis demonstrates that the plant remains commercially viable and profitable despite the incorporation of renewable feedstocks. The utilisation of corn stover reduces biomass waste and greenhouse gas emissions, lowers dependence on fossil resources, and supports local employment and supply chains. By embedding sustainability, safety, process integration, and economic assessment within a unified design framework, this work provides an industry-relevant and transferable model for low-carbon styrene manufacture aligned with UN Sustainable Development Goals 7, 12 and 13.

Keywords: sustainable process design; styrene production; bioethanol feedstocks; life cycle assessment; process integration



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1. Introduction

Styrene production is already a large and growing industry; the market stood at 42 million tonnes in 2024 and is forecast to grow at a Compound Annual Growth Rate (CAGR) of 4.37% until 2035 [1]. India is the largest importer of styrene in the world, with an estimated trade value of over 1 billion USD each year; therefore, it is the target country for this project [2]. Globally, conventional styrene production involves a two-step method: first, the Friedel–Crafts alkylation of benzene and ethylene to produce ethylbenzene, and second, either a catalytic dehydrogenation process or the styrene monomer/propylene oxide (SMPO) process is used to synthesise styrene. With rising climate change concerns due to greenhouse gases (GHG) and other forms of pollution, the 2015 Paris Agreement

was adopted to combat rising global temperatures, and the current conventional styrene production method is detrimental to achieving this goal [3]. This is largely due to the impacts of ethylene production and use. As a petrochemical sourced from fossil fuels, ethylene is a high carbon dioxide emitter and requires an energy-intensive process to crack from a mixture of hydrocarbons. Furthermore, ethylene and ethylene oxide are both air pollutants that can be released during industrial processes and adversely affect human health, causing issues such as respiratory problems.

This work evaluates the design, implementation, and feasibility of a styrene production plant, integrating established ethylbenzene dehydrogenation practices with innovative bio-catalytic feedstock processing, aiming to drive the transition to low-carbon, low-waste styrene production. Based on the Gujarat coastline of India, this innovative approach addresses environmental, social, and economic priorities while ensuring high efficiency and maintaining profitability to reduce reliance on fossil fuels. The current leading approaches for the biosynthesis of styrene involve the conversion of L-phenylalanine, derived from renewable sugars, into styrene via a two-step enzymatic pathway [4,5]. The proposed process capitalises on the fermentation of local corn stover to generate bioethanol, which then undergoes alkylation with benzene to produce ethylbenzene, which is subsequently converted into styrene. Not only is producing bioethanol this way a low-carbon alternative to the conventional method, but it also utilises an agricultural waste product, corn stover, instead of a non-waste product such as field corn, which is prominently used in the US to produce bioethanol [6]. In contrast to the approaches proposed by McKenna and Nielsen [4] and Spekrijse et al. [5], which use L-phenylalanine as the precursor, producing styrene via bioethanol derived directly from biomass enhances material integration by minimising waste generation, maximising the reuse of process streams, and recycling by-products for internal use or external valorisation. These strategies improve overall resource efficiency and contribute to the sustainability of the process.

2. Research Objectives

The primary objective of this research is to advance the sustainable production of styrene by utilising bioethanol derived from agricultural waste as a renewable feedstock. Specifically, corn stover is valorised through an integrated biorefinery approach, transforming an abundant lignocellulosic residue into a value-added chemical intermediate. This strategy demonstrates how agricultural waste can be effectively incorporated into industrial chemical production, thereby promoting sustainable processing across both the chemicals and bioenergy sectors. Furthermore, the study explores the practical implementation of comprehensive material integration to maximise resource utilisation, minimise waste generation, and enhance process efficiency. The proposed approach offers significant environmental, economic, and societal benefits, supporting the transition towards a circular and low-carbon chemical industry.

A notable objective within the project is the utilisation of the black liquor drained from the pretreatment reactor during the preparation of the feedstock. In industrial operations, it is more common to burn this liquor as a method of energy creation [7]. The project aims to maximise the potential use of this black liquor before it is burned for energy creation, maximising environmental sustainability while also carefully considering economic sustainability. Critically, we designed the process such that we can reuse the sodium hydroxide solution present within the liquor, reducing the amount of additional chemicals required to precipitate out lignin using carbon dioxide produced in the fermentation reactor, and recycling the precipitated lignin for industrial use, such as in construction, adhesives, and fuel/energy generation [8].

3. Styrene Production Processes

3.1. Conventional Styrene Production

There are two routine procedures used to synthesise styrene in industry: catalytic dehydrogenation of ethylbenzene to produce styrene, and the styrene monomer/propylene oxide (SMPO) process, where styrene is produced as a side product of propylene oxide. While these processes are not highly complex, they rely heavily on ethylene, a petrochemical that heavily contributes to air and water pollution, greenhouse gas emissions, and the release of harmful chemicals into the environment and consumer products [9]. The conventional method of producing ethylbenzene is Friedel–Crafts alkylation in the presence of a zeolite catalyst at temperatures of 150 °C to 450 °C. This process additionally produces diethylbenzene as a side product, which can undergo transalkylation to produce more ethylbenzene [10].

Catalytic dehydrogenation of ethylbenzene over a potassium-promoted iron oxide catalyst is the established industrial process for styrene production, owing to its high selectivity, catalytic efficiency, and suitability for large-scale continuous operation. This process has a selectivity of 96.2% at 560 °C and a steam-to-ethylbenzene ratio of 10:1 at atmospheric pressure [11]. This produces benzene and toluene as side products for recycling and sale, as well as regenerating process steam. Conversely, the Styrene Monomer Propylene Oxide (SMPO) is a copolymerisation process. Ethylbenzene is oxidised to ethylbenzene hydroperoxide (EBHP) using oxygen gas occurring in horizontal bubble columns, with any unreacted ethylbenzene being recycled back using a condensing column. The effluent is processed after neutralising acidic by-products [12]. Conditions for this reaction are a temperature range of 135–160 °C and a pressure range of 2.28–4.48 bar in the oxidative zones. The main by-products are methyl phenyl ketone (MPK), methyl phenyl carbinol (MPC) and a small number of carboxylic acids [13]. Propylene is fed into a reactor with the EBHP stream, where epoxidation of propylene by EBHP occurs using a fixed-bed reactor, producing propylene oxide and MPC. The reaction often occurs using a titanium-on-silica catalyst (Ti/SiO₂), resulting in an overall conversion of EBHP close to 100% and a selectivity of propylene oxide close to 95%. The conditions use a temperature range of 40–135 °C and a pressure range of 20–80 bar, with the by-products being phenol, aldehydes, and MPC [14]. Crude products require distillation to separate the unreacted reactants, MPC and MPK. Further purification of propylene oxide is required using azeotropic distillation [12]. MPC and MPK are subsequently fed into the reactor for dehydration, which converts MPC to styrene and water using a liquid catalyst of para- and ortho-toluene sulfonic acid. The conditions are 200–230 °C and 0.2–0.3 bar, achieving conversion rates up to 85% with 92% selectivity for styrene. The crude styrene is separated off and purified by distillation; vapours need to be scrubbed to remove the catalyst from the effluent. The leftover reactants are sent to the catalytic hydrogenation unit, where MPK reacts with a hydrogen source to form MPC. A Cu/SiO₂ catalyst can be used, with conversion and selectivity being over 95% [15].

3.2. Bioethanol as an Alternative Feedstock

Due to the environmental risks associated with using ethylene to promote sustainability, the proposed route uses bioethanol as a feedstock. This involves an additional multi-stage process to synthesise the bioethanol from agricultural waste, which presents a low-carbon alternative to the traditional route. Agricultural wastes such as rice straw, wheat straw, corn stover and sugarcane bagasse are conventional feedstocks due to their high cellulose and hemicellulose contents, all of which must undergo pretreatment processes for size reduction (milling) and lignin removal (chemical pretreatment to promote higher yields of bioethanol production [16]. Following this, enzymatic hydrolysis is required to

break down the polysaccharides (cellulose and hemicellulose) into their monosaccharides (glucose and xylose), which are sugars that can be fermented by bacterial strains into bioethanol. The bioethanol is then separated using a distillation column to produce a water–bioethanol distillate for use in the benzene alkylation process. Subsequently, the benzene and bioethanol are reacted to produce ethylbenzene, with a selectivity of 85.8% and conversion of 95% with respect to ethanol and using a beta-zeolite catalyst at 10–30 bar and 200–270 °C [17].

3.3. Advances in Biocatalytic Processing

The advancement of biological catalysts in the industrial sector has been paramount in developing highly sustainable and economically beneficial processes. The protein engineering field has continuously developed enzymes with high conversion rates and high specificity [18]. Enzymes typically also have mild operating conditions, leading to lower energy consumption, water usage, and raw materials, and producing less waste, all of which contribute to a more environmentally friendly process by preserving our natural resources and reducing emissions [19]. These developments have already made a significant impact, such as predictions that these efficiency improvements could save up to 139 MtCO₂e (MtCO₂e = million metric tons of carbon dioxide equivalent) in the food industry and up to 65 MtCO₂e in traditional industries [20]. The use of bacterial strains also provides similar benefits, where processes require less energy and produce fewer harmful by-products [21]. More recently, techniques have been developed through genetic engineering, such as random mutagenesis and genome editing, to modify these bacterial strains to further improve their functionalities [22]. Additionally, a major benefit of using bacteria for the process can be seen as ‘capital cost’, as the bacteria will grow and reproduce and would not need to be replaced, unlike standard metal catalysts.

3.4. Process Safety and Waste Management

3.4.1. Chemical Safety

The overall biomass-to-styrene process contains chemicals of high danger to humans and the environment. Styrene, ethylbenzene, benzene, bioethanol, toluene, sodium hydroxide, phosphoric acid, and hydrogen sulphide are all extremely toxic substances with a safe exposure limit of less than 1 g/m³ for humans and aquatic life. Many of these substances, especially styrene and ethylbenzene, have exceptionally low flashpoints of 23–31 °C. Consequently, they must be kept away from any sources of heat, flames, static electricity, or any ignition sources. Explosive vapour–air mixtures can spread across floors and underground areas. Ethylbenzene should be treated with extreme caution in handling and transporting, both of which should be kept to a minimum. Fires should be put out with sand or carbon dioxide, as any water used should not be allowed to drain anywhere else and could function as a spreading agent for the fire.

Keep containers closed and protected from sunlight, and any containers or receiving equipment should be grounded to prevent the build-up of static electricity. Explosion-proof electronics and non-sparking tools should be used. Workers should always wear gloves, eye protection, and skin protection barrier creams. Some chemicals used as intermediary products are highly carcinogenic, especially when mixed with dust or vapour. As a result of this, adequate ventilation for all individuals is essential, and in the case of dealing with benzene, toluene, and hydrogen sulphide, extra ventilation may be required, including process enclosures when dealing with the latter.

3.4.2. Material Incompatibility

Styrene, benzene, ethylbenzene, toluene, and hydrogen sulphide are all incompatible with oxidisers or oxidising agents, such as oxygen, ozone, hydrogen peroxide, potassium

nitrate, etc. Iron (III) oxide is incompatible with strong reducing agents. It presents the potential for hazardous explosive reactions with aluminium, calcium silicide, ethylene oxide, polymers, carbon monoxide, and magnesium perchlorates. There is a risk of ignition or formation of flammable gases or vapours with carbides, hydrogen sulphide, and hydrogen peroxide, as well as exothermic reactions with hydrazine hydrate and calcium hypochlorite. The β -zeolite catalyst is incompatible with strong acids, strong bases, hydrogen fluoride, chlorine trifluoride, ethylene oxide, halogenated hydrocarbons, oxygen difluoride, sodium nitrate, and vinyl compounds. Sodium hydroxide reacts violently with many chemicals, but the notable ones are water, organic substances, hydrogen sulphide, phosphorus oxides, halogenated hydrocarbons, light metals, metals, acetone, magnesium, zinc, and tin. Hydrogen sulphide and organic substances are of particular concern because they are found elsewhere in the process.

A chemical compatibility matrix can be found below (Table 1), which shows a complete breakdown of the dangerous reaction potential within the system, and in particular shows the necessity to remove any additives such as hydrogen sulphide due to its ability to react negatively with other compounds in the process. Furthermore, a risk matrix for the plant is shown to analyse the risk likelihood, impact, and recommended control measures for the chemical safety analysis shown above. The table displays (top to bottom) and (left to right) the amounts of the compound found in the process and the amount of heat or vigour of reaction displayed in green (no reaction or gentle reaction), orange (some reaction) or red (vigorous or heat-expelling reaction that could be dangerous).

Table 1. Chemical compatibility matrix.

	Styrene	Ethylbenzene	Benzene	Bioethanol	Steam	Iron (III) Oxide	Toluene	Carbon Dioxide	Sodium Hydroxide	Corn Stover	Phosphoric Acid	Beta Zeolite Catalyst	Hydrogen Sulfide	Carbon Monoxide
Styrene														
Ethylbenzene														
Benzene														
Bioethanol														
Steam														
Iron (III) Oxide														
Toluene														
Carbon Dioxide														
Sodium Hydroxide														
Corn Stover														
Phosphoric Acid														
Beta Zeolite Catalyst														
Hydrogen Sulfide														
Carbon Monoxide														

4. Design and Optimisation

4.1. Optimum Location—Gujarat, India

India currently produces high amounts of bioethanol, with amounts up to 1.3 billion litres from cane molasses [23]. The use of sugarcane should ideally be avoided, as is most evident in Brazil, where rainforests are being cut down for further production of sugarcane. This led to the decision to synthesise bioethanol from corn stover, as this is a waste product of agriculture rather than a food product. The composition of corn stover

varies significantly across different regions where it grows, but newly developed methods like ionic liquids show promising results for lignin degradation. In India, corn stover is primarily grown on the west coast, which solidified our choice to build the plant in Gujarat, a state located in the northwest of India, to take advantage of proximity to the corn fields. In 2024, the biggest importer of styrene was India, securing the first position, implying that India tends to import styrene rather than export it because it is consuming it for its relevant applications in producing plastics, synthetic rubbers, and foams [2]. Building the chemical plant in India ensures proximity to existing consumers, lower transport costs compared to importing overseas, as well as reduced GHG emissions.

Gujarat is an excellent hub for infrastructure with its great transportation options all close by, including ports and airports, as well as roadway networks spanning over 74,000 km and 5310 km of rail lines, which will be beneficial for keeping import and export prices as low as possible. Gujarat also takes pride in its robust power generation, where its hydroelectric projects have been well developed, contributing to its renewable energy sources. Currently, corn stover is often burned in fields, although it is a significant agricultural residue, given that the world supply of corn stover can be used to produce over 45 million cubic metres of bioethanol—approximately 60% of world production. This shift would reduce GHG emissions by over 150 million metric tons of CO₂ equivalents annually. This aligns well with India's ambition for carbon neutrality by 2070, with a 50% reduction by 2030, as well as contributing towards goals set in the 2015 Paris Agreement [3].

4.2. Feedstock Selection and Pretreatment

To maximise sustainability goals, bioethanol is synthesised from an agricultural waste, corn stover, to be used in the main process. This is because cellulose and hemicellulose comprise 70% of corn stover, which can be converted into bioethanol [24]. Additionally, India has a high abundance of corn stover waste alone to fuel the process, as it is estimated that India produces 42 million tonnes of corn per annum [25]. The pretreatment process is the most crucial step to achieve high yields of bioethanol, as lignin acts as a barrier that protects the cellulose and hemicellulose we want to access. Therefore, we follow a process proposed by the Royal Society of Chemistry to achieve high lignin removal and low cellulose/hemicellulose loss [26]. The corn stover (at an input size of several cm) must first be knife milled to reach a uniform size that allows it to pass through a 19 mm round-hole screen, ensuring that the stover is uniform enough for the upcoming alkali treatment, as larger sizes could reduce deacetylation efficiency. The alkali pretreatment involves the knife-milled biomass being mixed with a dilute sodium hydroxide solution in a ratio of 20 g of corn stover per 160 mL of 2% NaOH solution at 80 °C for 2 h, as this will remove acetyl groups and begin to break down the lignin structure to expose the cellulose and hemicellulose in the corn stover [27]. However, due to the extraction technique, about 2.8% and 33.5% of the cellulose and hemicellulose, respectively, are diluted by sodium hydroxide, although the benefit of removing 73.9% of the lignin far outweighs this loss [27]. The residual liquid is then drained, and the solids are washed to remove excess sodium hydroxide solution (0.1 M NaOH, about 4 g of NaOH per litre of water). The drained liquor is then put through a separation process to recover the sodium hydroxide, which can be recycled, and the lignin, which can be sold. Before the next step, the pH must be adjusted to maximise both the hydrolysis and the fermentation. This is done by adding dilute hydrochloric acid, controlled by a pH control loop, to the solids to reduce the pH to around 5, which is the compromised pH for the future saccharification and fermentation process. The slurry is then passed through a screw press, which dewateres about 45–50% of the water, as it is much easier to mill a dry product than a wet product. Further mechanical refining is then performed in the form of disc refining and Szego milling, as this will break

down the structural integrity of the corn stover to increase its surface area and make the cellulose and hemicellulose more accessible to increase the sugar yield for the two-phase simultaneous saccharification and fermentation (TPSSF).

TPSSF is the use of a single two-phase process that improves the efficiency of converting the pentose and hexose sugars to bioethanol within a single-reactor system. This achieves a high conversion of both polysaccharides and sugars, while also reducing the need for multiple reactors, as separate saccharification and fermentation reactors are not required. This method also minimises by-products and maximises the overall yield of bioethanol to be around 84% [28]. The process first involves the use of enzymatic hydrolysis using enzyme blends provided by Novozymes; these are the Cellic[®] CTec 3 and Cellic[®] HTec 3. These enzyme blends contain both cellulases and hemicellulases, which break down the cellulose and hemicellulose into oligomer forms such as cellobiose and cello-triose. The oligomers are then hydrolysed further by these enzymes into their respective monosaccharides: glucose (cellulose) and xylose (hemicellulose). The expectation is that 90.7% of the cellulose and 94.9% of the hemicellulose are converted into their respective monosaccharides [28]. Once the glucose and xylose sugars have been released, the bacteria can now begin fermenting these sugars into the bioethanol product. Due to having both hexose and pentose sugars in this reactor, different microorganisms are required to ferment each sugar, including *Saccharomyces cerevisiae* D5A and *Escherichia coli* KO11. Both bacterial strains fit the conditions, as well as having comparable pH and temperature ranges to work effectively with the enzyme blends, for which a pH of 5 and a temperature of 37 °C is the optimal compromise [28]. These bacterial strains will be grown in separate fermenters beforehand to keep a constant supply. From the amount of cellulose and hemicellulose converted into their sugars, the assumption is made that 46–49% of the sugars are converted into bioethanol and the carbon dioxide by-product [28]. After the reaction time has been completed, the slurry is passed through a centrifugal separator to remove any remaining solid waste, such as the residue lignin, cellulose, hemicellulose, enzymes, and bacteria, to leave just a solution consisting mostly of bioethanol and water. The solid waste stream is used to recover the enzymes, and the remaining solid is separated and dried to be sold as animal feed. For the bioethanol solution, distillation is required to purify the bioethanol from the water and other by-products that may have formed. Since the boiling point of ethanol is 78.37 °C, that would be a suitable temperature for this distillation, as pure ethanol is not required in this scenario. Many reactions use anhydrous ethanol, which would require further and more expensive purification. However, in the subsequent reaction with benzene, ethanol with a water content up to 20 w/w% can be used, but ideally 5%.

Within the bioethanol section, material integration has been heavily facilitated, resulting in many environmental and economic benefits. The first of these is the utilisation of the black liquor that drains out of the pretreatment reactor, which is common in biorefinery industrial processes where this liquor is burned to create energy; however, it is possible to utilise the black liquor further [7]. First is the recovery of the sodium hydroxide solution, which can be recovered by using a size exclusion methodology due to the varying size of species present in the black liquor. A size exclusion chromatography column is used with the ultra-high crosslinked non-ionic microporous resin Mn270 as the adsorbent, and the eluent is water [29–31]. This method is especially favourable not only for the high recovery rates of both the sodium hydroxide and lignin but also due to the strong physical and chemical properties of the MN270 resin, resulting in it not requiring replacement [32]. The mechanism of this separation is simple: the sodium hydroxide is small enough to enter the resin pores, while the larger lignin molecules cannot. After the black liquor passes through the column, water can then be flushed through the column, releasing the NaOH solution from the pores, which can then be collected in a separate container to form the

liquor. The high recovery rate is not only due to the size exclusion but also the interaction between the lignin and resin itself, where the lignin acts as a facilitator that promotes further NaOH–resin interactions [29]. With the NaOH solution now separated from the remaining black liquor, we can evaporate off the eluent water used in the chromatography column to achieve a 2% sodium hydroxide solution to be reused in the pretreatment reactor.

The remaining black liquor is not forgotten, as it is possible to process this further to result in a dried product containing mostly lignin, which has a multitude of uses and can be sold [33]. The method chosen for this is to precipitate the lignin out of the black liquor, which involves reducing the pH, typically using a strong acid. Using an acid is not the only way to reduce the pH; carbon dioxide can be used, and the two-phase simultaneous saccharification and fermentation reactor produces this carbon dioxide as the sugars are fermented into ethanol and CO₂ [33–36]. This way not only is there a recovery of lignin, but the remaining black liquor is being used as a method of carbon capture by carbonation, significantly reducing our emissions of greenhouse gases [37]. This reaction is performed at ambient temperature and pressure, where the carbon dioxide is bubbled through the black liquor, causing a reduction in pH and the formation of sodium carbonate and decarbonate [7,38]. The slurry is then separated using a centrifugal separator to remove the sodium carbonates/decarbonate solution so that it can be washed, dried and sold.

The final material integration is implemented after the TPSSF reactor, using the solid waste separated from the ethanol mixture. This solid waste contains the enzymes used previously in the reaction, which are to be recycled since they can be reused continuously, saving on the cost of the enzyme blends. The focus here is more on conserving the enzymes because, while it could be beneficial to also try to separate the bacteria, the bacteria can easily be grown in fermenters, whereas the enzymes cannot reproduce due to not being microorganisms. In this case, ultrafiltration was chosen as the method to separate the enzymes from the mixture due to the scalability of the process, and the membranes used can easily be swapped out and cleaned to maximise efficiency [39–42]. While the initial investment for this equipment is high, it will save a significant amount of cost overall as fewer enzymes need to be purchased, thereby reducing our operating costs. Following the enzyme separation, to make use of the remaining solid waste, it is proposed that, since we are taking away a source of animal feed by using corn stover, the effect of this should be mitigated [43]. Therefore, evaporating the stream followed by a drying process to remove water is a suitable method to acquire dried solid waste, which can then be used as animal feed.

4.3. Ethylbenzene Synthesis, Ethylbenzene Side Product Recovery

Bioethanol is used in a reaction with benzene to form the intermediate ethylbenzene (EB) for making styrene. At first, the method chosen had a selectivity of 85.8% to ethylbenzene and aromatic conversion of 95% with respect to the bioethanol under the optimum conditions of using a BEA-type catalyst, which exceeded the 83% selectivity associated with conventional practice [44,45]. A temperature of 240 °C to 260 °C and a molar ratio of benzene-to-ethanol of 2.5 were used with an operating pressure of 25 bar, so that reactive distillation would be possible. Reactive distillation was changed to a PFR to reduce complexity, with the pressure remaining the same for the process in the group section. However, optimisation of pressure for this was considered in detail. These conditions also reduced the unwanted by-products, which are polyethylbenzenes, which can undergo transalkylation to process them into ethylbenzene to increase the yield. At 270 °C, the transalkylation of diethylbenzene over a BEA-type catalyst has a selectivity of 96% with a 40% conversion per pass [46]. Separation of all streams is done using distillation, with the

recycle stream of the alkylation reactor requiring extractive distillation to remove excess water from the stream.

The selectivity of ethylbenzene synthesis in the packed-bed reactor was systematically assessed using Aspen Plus by performing a detailed sensitivity analysis. This approach facilitated the identification of critical operating parameters governing reactor performance and product selectivity, providing a robust basis for process optimisation and improved process efficiency. Sensitivity analysis in Aspen Plus is a systematic method used to determine how changes in specific input variables affect process outputs, performance metrics, or economic indicators. Results revealed non-linear and interdependent relationships among variables. For example, temperature increases improved conversion but raised energy costs and side product formation. Economically, variations in ethanol cost significantly altered profitability, marking it as a high-sensitivity input. The outputs helped identify safe operating envelopes and informed control setpoints. Aspen Plus has a significant role in reactor design. Sensitivity analysis ensured robustness in reactor design by evaluating a range of realistic operating scenarios. It supported decision-making for control strategies, sizing of equipment, and contingency planning. Additionally, it highlighted parameters for which tight operational control is necessary.

Overall, the observations from the sensitivity plots confirmed that there must be a compromise on getting the selectivity higher than a certain extent, as keeping the costs reasonable as well as the process safe enough needs to be prioritised. After careful consideration of all the graphs generated from Aspen Plus and MATLAB R2021a, the decision was made to settle on the operating conditions that would allow the pressure to be within safe limits and a reasonable temperature and catalyst weight to control the production costs.

In the proposed sustainable styrene production pathway, ethylbenzene (EB) is synthesised via the liquid-phase alkylation of benzene with bioethanol, catalysed by beta-zeolite under moderate pressure and elevated temperature conditions (typically $\sim 200^\circ\text{C}$, 5 bar), resulting in a selectivity of ethylbenzene in the reaction to be 85.8% [44]. The process is exothermic and benefits from high benzene-to-ethanol molar ratios to maximise monoalkylation and suppress polyalkylation. However, side reactions lead to the formation of minor by-products such as diethylbenzene (DEB), toluene (via ethanol dehydration to ethylene followed by Friedel–Crafts alkylation), and trace unreacted ethanol. These components are separated via a downstream distillation train, where DEB is selectively removed and recycled or cracked back into EB, while excess benzene is recovered and fed back into the reactor. Toluene, present in small quantities, may be separated as a secondary product for sale or solvent use, contributing to process value recovery.

Following the styrene section of the plant, unreacted benzene is continuously recycled through a loop system, improving atom economy and reducing raw material costs. The alkylation unit is thermally coupled with pre-heaters and heat exchangers to minimise energy demand by recovering heat from exothermic reaction zones and integrating it with upstream feed preheating and downstream distillation operations. Moreover, ethanol sourced from the TPSSF unit is directly fed into the alkylation reactor after purification, maintaining feedstock continuity and reducing storage requirements. This interconnected approach improves mass efficiency, reduces waste generation, and enhances the overall sustainability of the styrene synthesis train.

As a process, the synthesis of intermediate ethylbenzene uses an acylation and transalkylation reactor. This is due to the selectivity of ethylbenzene in the acylation reactor, with a considerable proportion of the products being diethylbenzene. This can be separated off and reacted with benzene in the transalkylation reactor to form ethylbenzene. This increases the overall efficiency and selectivity of the process, reducing the amount of waste product produced.

The process water removed through extractive distillation is at a high purity above 99.99%; there are small levels of glycerol, ethanol, and benzene impurities; however, they should be below the acceptable levels in normal operation. The aromatics in that wastewater were 0.04 ppm, significantly below the 0.1 ppm required before discharge, and the ethanol released is at 1.7 ppm, requiring an oxygen demand of 3.55 ppm, below the 15 ppm for biochemical oxygen demand (BOD) [47]. At the rate at which it is produced, it would allow for process water to be replaced regularly, reducing the build-up of impurities in the system. This water is likely to be purer than process water, which would be brought in since it has been distilled, so it would have less ionic and organic content. For safety reasons, testing would be used to ensure that it is up to standard before any water is released into the environment or used for process streams.

4.4. Styrene Production, and Styrene Side Product Recovery

Catalytic dehydrogenation of ethylbenzene to produce styrene is a widely used and well-optimised process [48]. The main responsibility of the packed bed reactors is to produce the saleable styrene monomer (SM) and toluene from the ethylbenzene (EB) created. Catalytic dehydrogenation of EB to produce SM is a widely used and well-optimised process, with the iron oxide catalyst (IOC) accounting for 85% of commercial production [48,49]. Elevated temperatures of 560 °C and low adiabatic pressures of 2.7 bar are required due to the reversible, potassium-promoted iron oxide-catalysed reaction, and work best when mixed with steam to lower the ethylbenzene partial pressure inside the vapour-phase reactors. Excess side reactants are formed under higher temperatures and partial pressures, such as benzene, toluene, ethylene, and carbon dioxide.

The process uses two adiabatic gas-phase reactors in series; the first is optimised and designed in detail (diameter 4.3 m, length 17.3 m), with a furnace heating in between to maintain the endothermic reaction heat. The process inlet stream starts at 487 °C with 639 kmol/h (52% recycled) ethylbenzene and 5000 kmol/h low-pressure pre-heated process steam, increasing the total temperature to 560 °C. The output SM (283 kmol/h per pass) and by-products enter a decanter at 40 °C after cooling in a heat exchanger [50]. The remains after water removal are purified through distillation columns for sale as toluene or to recycle the EB, and maintain over 87% total yield, as without EB recycling to maintain a constant yield, the flow rate of benzene entering the reactor would be 711 kmol/h [48]. Overall, 286 kmol/h is created in the plant, which is a 6% margin over the necessary 220 ktonnes per year. Nominal purity rates are currently 99.7%, which is the ASTM D2827-00 standard [51]. The purity of styrene is checked in this process through a gas chromatography check on the output of the relevant distillation column, which was the alternative to the freezing point method used in ASTM D3799-95 [49].

While vertical reactors are also commonly used for packed beds, nominally due to their ease of catalyst loading and predictable gravitational effects on particle distribution, a horizontal PBR was chosen for this design element. This is primarily because of the size, meaning that improved temperature control and uniform flow distribution are more important than normal to avoid wasting catalyst due to hotspots and to maintain high selectivity, which would otherwise increase recycling costs.

The reaction kinetics used for the reactor are a development of Langmuir–Hinshelwood–Hougen–Watson kinetics (LHHW), modelled as four reactions, the first being reversible EBSM and the side reactions to produce benzene/ethane and toluene/methane. This was chosen to account for the adsorption and desorption of the reacting species with accuracy in ASPEN, to allow for sensitivity analysis to optimise process variables. Temperature optimisation for economics and outputs advised that although the reaction goes closer to competition per pass at higher temperatures, decreasing the reactor inlet tempera-

ture decreases net expenses, which pays off against the increased recycle ratio (660 °C to 560 °C) [48]. Utilisation of the post-process heat was repurposed to run distillation columns and heat EB production via heat integration. The toluene that is distilled can also be sold.

Steam flow rate was optimised to balance competing demands on selectivity and flow rate while minimising furnace expenses across the system. Excess steam acts as a cost-effective process heater that decreases EB partial pressure and variably shifts reaction equilibrium via prevention of carbonaceous deposits within the 6–18:1 steam ratio; therefore, the steam ratio was chosen to be 7:1 (5000 kmol/h) [52].

Similarly, there was a fine balance in the initial pipe pressure regarding optimal space velocity (919 h^{-1}) and pressure drop across the packed bed. Pressure drop minimisation to below 1 bar (0.77 bar) was essential in preventing physical degradation of the catalyst, while balancing a minimal reactor volume (188 m^3). A packed-bed reactor was chosen to prevent excessive voidage variations across the reactor [53]. The inlet velocity was diffused across three 815 mm pipes from 25 m/s to 10 m/s with a diffuser angle of 7° to prevent excessive backflow or eddy currents, which minimises coking in the centre bed [54,55].

Potassium ferrite (KFeO_2) was chosen as a catalyst promoter because of its ability to allow for continued self-regeneration of the iron oxide catalyst (IOC) without compromising activity levels at lower steam-to-hydrocarbon ratios required in the reactor design ($<11.8:1$). The dynamic equilibrium coke model found potassium suppresses the carbonaceous deposits via gasification mechanisms [56]. The volatility of potassium compounds creates a tendency to move, both with the fluid flow and inside the pellet due to the endothermic temperature gradient of the reaction, resulting in potential loss of activity and selectivity [57,58].

The catalyst weight per reactor was increased by 11% to 268,000 kg, increasing the styrene output per pass by 5% while functionally maintaining the selectivity (within 0.2%). The packed bed catalyst placement inside the reactor is contained in a mesh, with IOC pellets of voidage 0.43, diameter 5.5 mm, integrated with the potassium ferrite (KFeO_2) promoter. A larger pellet diameter is beneficial for cost savings compared to a 0.7 mm pellet, which is affected by the internal diffusion limit on the apparent activation energy (63 kJ/mol, formerly 96 kJ/mol, latter) [59].

The output styrene and by-products enter a decanter at 40 °C after cooling in a heat exchanger [50]. Water is withdrawn from the bottom of the process, and gaseous products leave for the distillation column. The bottoms of this distillation are fed into a second recycle column to remove the ethylbenzene to less than 1% of the second bottoms and less than 1% toluene for the distillate. Many optimisations to improve these numbers have taken place, including increasing the flow rate of steam, decreasing the reactor inlet temperature, increasing the reactor height and length, and considering the number of reactors.

Hydrogen is produced as a side product in the catalytic dehydrogenation reactor, where 319.46 kmol/h are separated using a decanter. This stream should be mixed with the natural gas used for the fired reboilers and furnaces to reduce the amount of natural gas required for the plant, thus lowering the overall carbon emissions. Separation and sale of this hydrogen were considered, but were rejected due to the complexity and costs associated with purification and the clear environmental benefits of utilising it as a fuel. Toluene and benzene are also by-products from the catalytic dehydrogenation reactor; the toluene was purified to 96% purity so that it can be sold as commercial-grade toluene, with the benzene being recycled to a prior section of the process. 95–99% was taken as commercial-grade toluene; the amount of ethylbenzene will need to be considered, as it will reduce the use cases [60].

4.5. Heat Integration

The styrene production side of the process plant is complex, with significant ranges in pressure and temperature being used; the integration of streams and utility loops was considered in this design to reduce cost and waste heat.

The process flow diagram, Figure 1, includes a representation of all the heat exchangers within the system; this PFD is limited in its detail, showing the positions of utilities, ignoring the connections, with some heat exchangers being representative of a chain, as can be seen for stream B34, where one heat exchanger is representative of five. This was done for simplification purposes, with the PFD in this section giving a broader discussion of the network designed. However, this section still uses some simplifications, with the CON_PXX and RB_PXX being representative of the condensers or reboilers from distillation columns, where the pressure of water is optimal, with XX being the pressure given in bar.

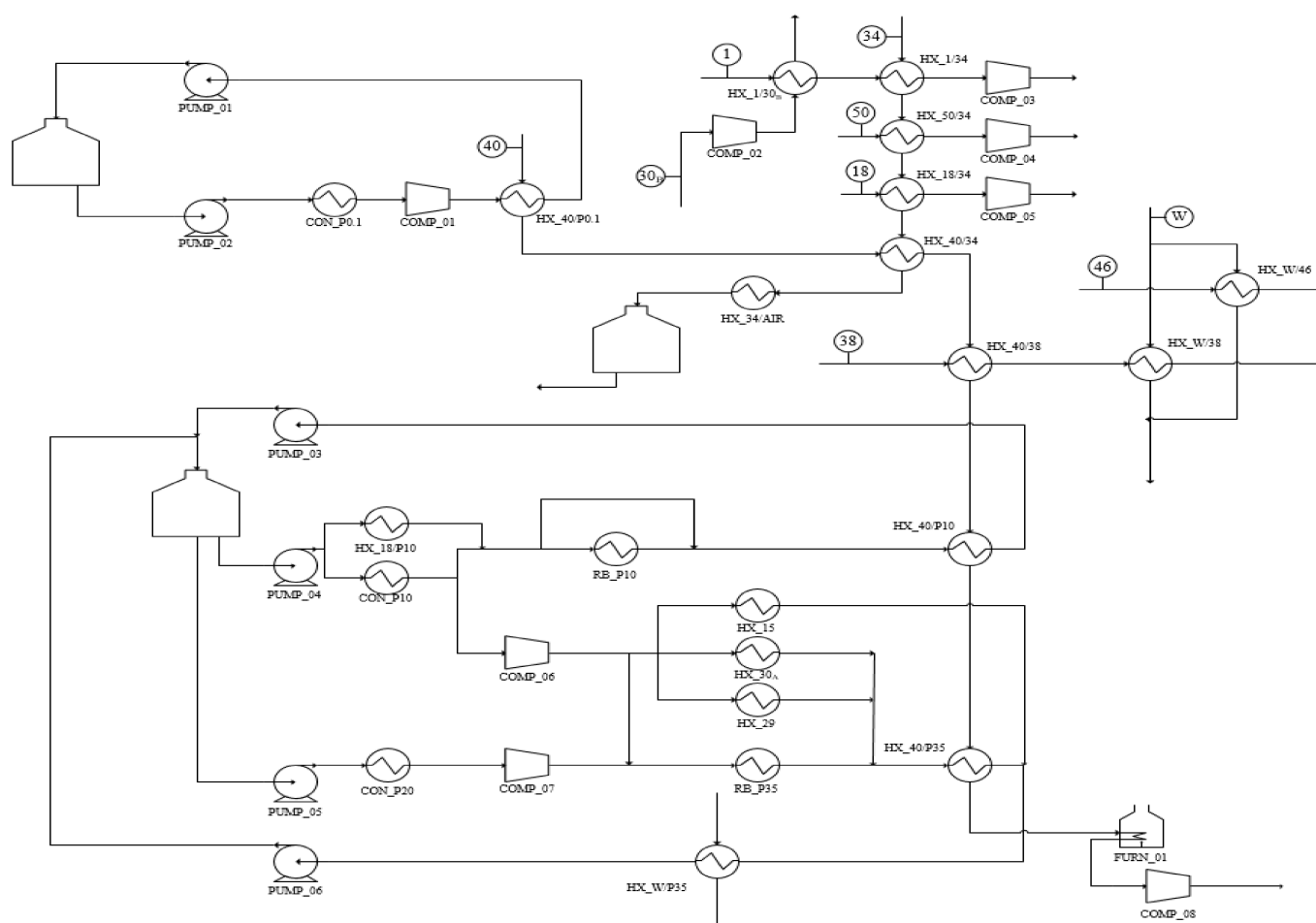


Figure 1. Process flow diagram for the heat integration system.

The cooling water pressure used was higher than would be required to obtain a higher-pressure stream from the condensers, as this is a more useful form of energy, reducing the need for compressors and thereby reducing electricity requirements. Higher-pressure steam is more useful in this case as it has higher boiling points, allowing for more flexibility when using it as a heat source for streams and reboilers, as much of the useful energy is in the latent heat of the water. The reboilers not discussed in this section used fired reboilers due to the high-temperature requirements, with comparable steam-based options requiring much higher pressures than those used for the integration process.

Figures 1–3 present the process flow diagrams for the heat integration system, the bioethanol production plant, and the styrene production plant, respectively. Figure 1 shows the connections and positions of the relevant components, with HX_XX or HX_XX/XX giving the relevant streams, with XX representing the heat exchanger for that stream, as seen in Figure 3, with A and B used to distinguish between the first or second heat exchanger, if necessary XX/XX is used for cases where both streams are not part of the utility loops, with the streams from Figure 3 being labelled with the same numbering.

There are two utility loops used for this process: the top loop, being the low-pressure loop initially at 0.1 bar, is used to cool the lower-pressure distillation columns, with the pressure needing to be low to be used efficiently for the condensers labelled by CON_P0.1, the process steam produced is increased in pressure to 2 bar so that it can be used to heat stream B40, and this allows the steam to be condensed and cooled back down to its initial temperature. The high-pressure loop is used to service the higher temperature and pressure streams, which includes process water/steam at 10, 20, and 35 bar to allow for this. Similar to the low-pressure loop stream, B40 is used to cool the process steam; however, due to the high pressure, the streams are condensed primarily using the reboilers. For the final cooling, done using stream B40 due to the position of the process streams in the chain of heat exchangers, the temperature is only reduced to 170 °C, which is below the boiling point temperature at 10 bar; however, it is at a much higher value than the low-pressure process stream. Further cooling is possible but unnecessary, as the high-pressure utility loop is designed with the high initial feed temperature in mind, allowing the loop to be circular. However, this would need consideration for the start-up process since the feed temperature would be closer to room temperature, which would affect the optimal flow rates used until the stored water reaches a stable temperature.

The process produces more thermal energy than it requires, mostly due to the use of fired reboilers and furnaces required for higher-temperature heating, because these external utilities are required to cool the process. Stream B34 uses an air-cooled heat exchanger to decrease the temperature below the threshold for the release of water. Similarly, streams B38, B46 and B35 require further cooling, with process water being used from nearby bodies of water, the water of which can only be increased by 7 °C. This requires large heat exchangers to allow for the high flow rates of process water to remain within regulations [47].

4.6. Process Flow Diagrams and Material Balances

This section presents the process flow diagrams for the heat integration system, the bioethanol plant, and the styrene production plant, together with the corresponding material balances for the bioethanol and styrene processes. Tables 2–6 present the material balances for the bioethanol and styrene production processes, with Tables 2 and 3 corresponding to the bioethanol plant and Tables 4–6 to the styrene plant.

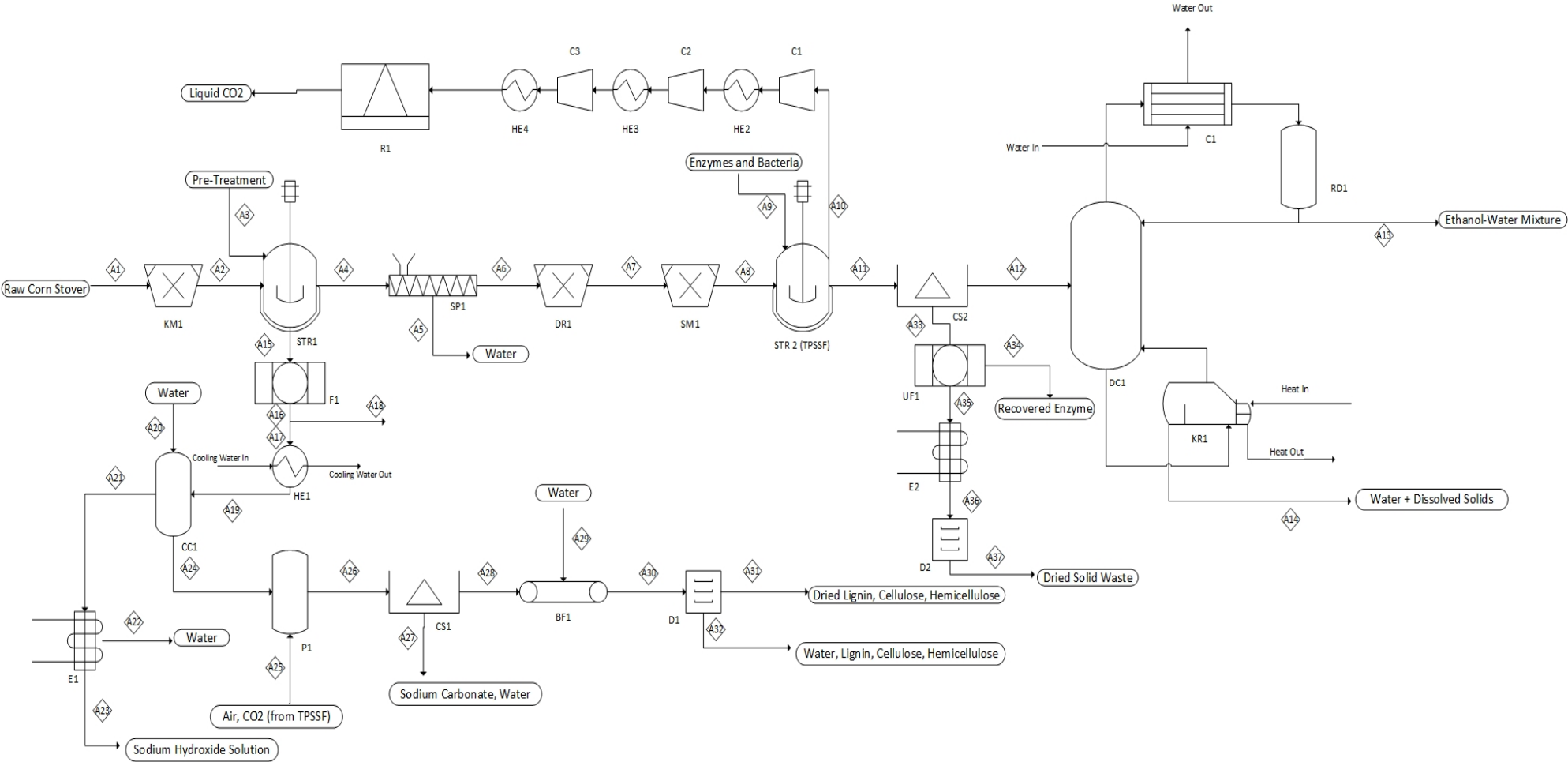


Figure 2. Process flow diagram for the bioethanol plant.

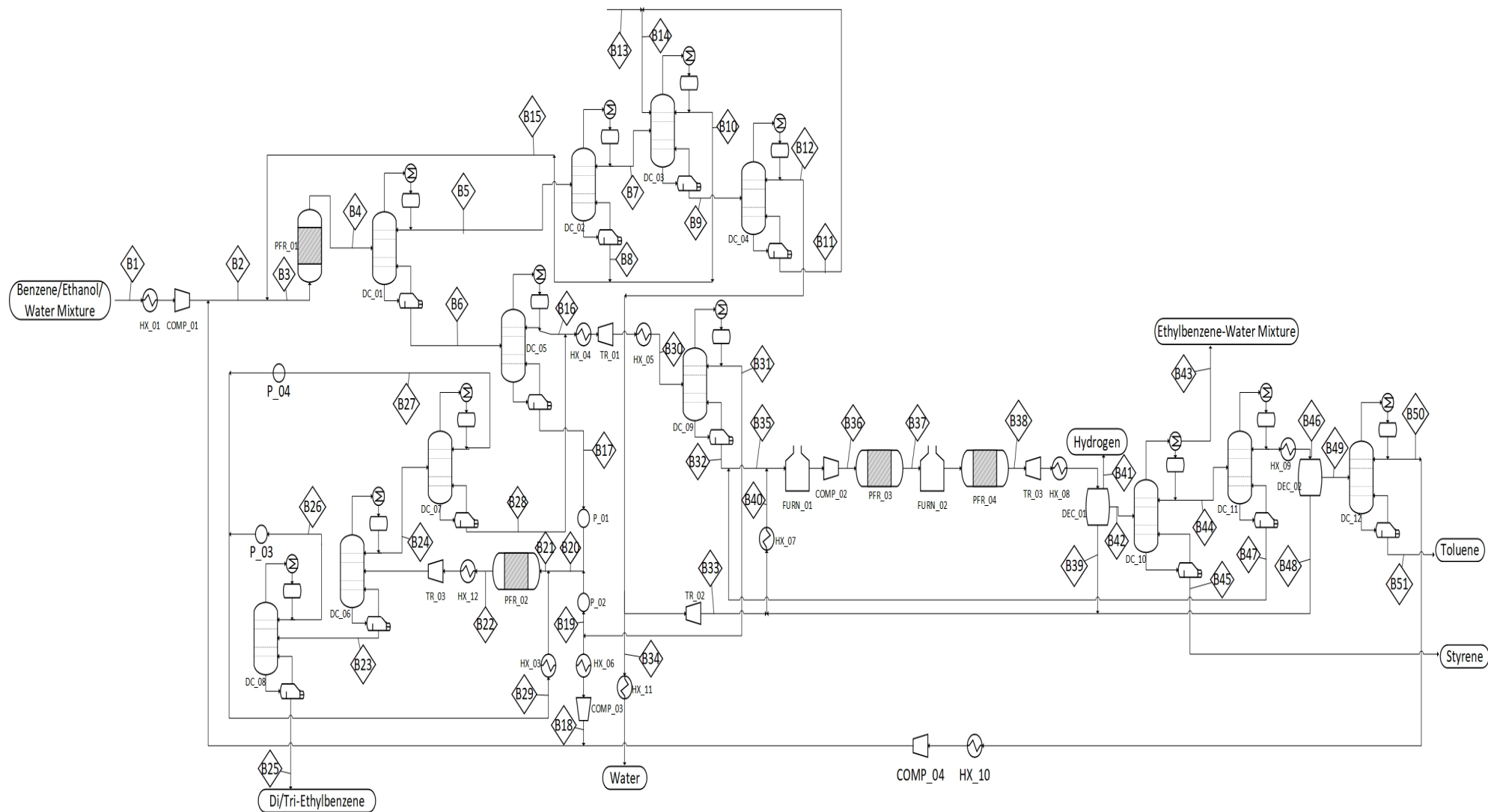


Figure 3. Process flow diagram for the styrene plant.

Table 2. Bioethanol material balance 1.

Species	Stream Flow (t/h)																	
	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18
Corn Stover	60.7	60.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH Solution	-	-	9.7	-	-	-	-	-	-	-	-	-	-	-	9.7	9.7	9.7	-
Water	-	-	910.4	151.7	96.3	55.4	55.4	55.4	162.6	-	15.7	15.4	1.0	14.4	758.7	758.7	-	758.7
HCl Solution	-	-	As Req.	-	-	-	-	-	-	-	-	-	-	-	-	-	-	As Req.
Lignin	-	-	-	3.1	-	3.1	3.1	3.1	-	-	3.1	0.06	-	0.06	8.6	8.6	8.6	-
Cellulose	-	-	-	22.8	-	22.8	22.8	22.8	-	-	2.1	0.04	-	0.04	0.7	0.7	0.7	-
Hemicellulose	-	-	-	11.0	-	11.0	11.0	11.0	-	-	0.6	0.01	-	0.01	3.7	3.7	3.7	-
CS Solid	-	-	-	12.3	-	12.3	12.3	12.3	-	-	12.3	0.2	-	0.2	-	-	-	-
Cellic CTec3	-	-	-	-	-	-	-	-	0.3	-	0.4	0.007	-	0.007	-	-	-	-
Cellic Htec3	-	-	-	-	-	-	-	-	0.09	-	0.09	0.001	-	0.001	-	-	-	-
<i>S. cerevisiae</i>	-	-	-	-	-	-	-	-	27.6	-	0.0005	0.000009	-	0.000009	-	-	-	-
<i>E. coli</i>	-	-	-	-	-	-	-	-	24.0	-	0.0004	0.00000008	-	0.00000008	-	-	-	-
Glucose	-	-	-	-	-	-	-	-	-	-	10.86	0.2	-	0.2	-	-	-	-
Xylose	-	-	-	-	-	-	-	-	-	-	5.5	0.1	-	0.1	-	-	-	-
Ethanol	-	-	-	-	-	-	-	-	-	-	14.8	14.5	14.5	-	-	-	-	-
CO ₂	-	-	-	-	-	-	-	-	-	14.1	-	-	-	-	-	-	-	-
NaCO ₃	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	60.7	60.7	920.1	200.9	96.3	104.6	104.6	104.6	214.5	14.1	65.3	30.6	15.5	15.1	781.5	781.5	22.8	758.7
Stream Temperature (°C)	30	30	30	80	30	30	30	30	30	30	33	33	33	33	99.1	78.2	30	30
Stream Pressure (atm)	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table 3. Bioethanol material balance 2.

Species	Stream Flow (t/h)																		
	A19	A20	A21	A22	A23	A24	A25	A26	A27	A28	A29	A30	A31	A32	A33	A34	A35	A36	A37
Corn Stover	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH Solution	9.7	-	9.6	-	9.6	0.1	-	0.009	-	-	-	-	-	-	-	-	-	-	-
Water	-	22.8	22.8	22.8	-	-	-	0.002	0.002	0.00004	4.3	4.3	0.3	4.0	0.3	-	0.3	0.02	0.5
HCl Solution	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Lignin	8.7	-	-	-	-	8.7	-	8.7	0.2	8.5	-	8.5	8.1	0.4	3.0	-	3.0	3.0	3.0
Cellulose	0.7	-	-	-	-	0.7	-	0.7	0.01	0.7	-	0.7	0.6	0.03	2.0	-	2.1	2.1	2.1
Hemicellulose	13.7	-	-	-	-	3.7	-	3.7	0.07	3.7	-	3.7	3.4	0.2	0.6	-	0.6	0.6	0.6
CS Solid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	12.1	-	12.1	12.1	12.1
Cellic CTec3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.4	0.3	0.07	-	-
Cellic HTec3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.09	0.07	0.01	-	-
<i>S. cerevisiae</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.0005	-	0.0005	-	-
<i>E. coli</i>	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.0004	-	0.0004	-	-
Glucose	-	-	-	-	-	-	-	-	-	-	-	-	-	-	10.6	-	10.6	10.6	10.6
Xylose	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5.4	-	5.4	5.4	5.4
Ethanol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.3	-	0.3	0.3	0.3
CO ₂	-	-	-	-	-	-	14.1	-	-	-	-	-	-	-	-	-	-	-	-
NaCO ₃	-	-	-	-	-	-	-	7.06	7.06	0.1	-	0.1	-	-	-	-	-	-	-
Total	22.8	22.8	32.7	22.8	9.6	9.6	14.1	20.1	7.3	12.9	4.3	17.2	12.4	4.6	34.8	0.36	34.4	34.0	34.5
Stream Temperature (°C)	80	40	30	40	30	30	30	30	30	30	105	90	30	75	40	35	35	35	35
Stream Pressure (atm)	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table 4. Styrene Material Balance 1.

Species	Stream Flow (kmol/h)																	
	B1	B2	B3	B4	B5	B6	B7	B8	B9	B10	B11	B12	B13	B14	B15	B16	B17	B18
Ethanol	313.24	313.24	1879.42	1566.18	1566.18	-	1321.03	245.16	-	1321.03	-	-	-	-	1566.18	-	-	-
Benzene	303.71	312.80	4676.91	4385.75	4364.12	21.64	665.56	3698.56	-	665.56	-	-	-	-	4364.12	21.64	-	2.92
Water	48.08	49.01	183.00	496.23	496.23	-	495.68	0.56	374.80	133.43	12.55	362.25	-	12.55	133.99	-	-	-
Ethylbenzene	-	-	4.26	273.02	4.26	268.76	-	4.26	-	-	-	-	-	-	4.26	263.38	5.38	-
Diethylbenzene	-	-	-	20.11	-	20.11	-	-	-	-	-	-	-	-	-	0.20	19.91	-
Styrene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Glycerol	-	-	-	-	-	-	-	-	600.00	-	600.00	-	-	600.00	-	-	-	-
Hydrogen	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Carbon Dioxide	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ethylene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Methane	-	-	0.79	0.79	0.79	-	0.79	-	-	0.79	-	-	-	-	0.79	-	-	-
Xylene	-	-	-	0.13	-	0.13	-	-	-	-	-	-	-	-	-	0.13	-	-
Toluene	0.08	0.25	1.64	2.31	1.39	0.92	-	1.39	-	-	-	-	-	-	1.39	0.92	-	-
Triethylbenzene	-	-	-	1.23	-	1.23	-	-	-	-	-	-	-	-	-	-	1.23	-
n-Propyl benzene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1,1-diphenylethane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1,2-diphenylethane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Butyl benzenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Heavies	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	661.76	670.81	6698.21	6697.96	6387.08	310.87	2465.42	3921.67	972.15	2105.73	612.46	359.69	0.00	612.46	6027.40	284.26	26.61	1.78
Temperature inlet (°C)	30	260.05	236.40	260.02	203.25	312.51	193.08	227.16	337.21	193.58	476.49	224.04	-	476.49	209.78	309.75	364.08	79.72
Pressure inlet (bar)	1	25	25	25	25	25	25	25	25	25	25	25	-	25	25	25	25	1

Table 5. Styrene material balance 2.

Species	Stream Flow (kmol/h)																	
	B19	B20	B21	B22	B23	B24	B25	B26	B27	B28	B29	B30	B31	B32	B33	B34	B35	B36
Ethanol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Benzene	23.49	23.49	586.39	568.59	-	568.59	-	-	562.91	5.69	562.91	27.33	26.41	0.92	-	-	0.92	0.92
Water	-	-	-	-	-	-	-	-	-	-	-	-	-	-	19.76	342.49	-	9265.58
Ethylbenzene	0.00	5.38	7.47	42.11	1.68	40.43	-	1.68	0.40	40.02	2.09	303.40	0.00	303.40	-	-	639.71	639.71
Diethylbenzene	-	19.91	45.11	27.06	26.71	0.35	1.51	25.20	-	0.35	25.20	0.55	-	0.55	-	-	0.55	0.55
Styrene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3.85	3.85
Glycerol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Hydrogen	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Carbon Dioxide	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ethylene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Methane	-	-	0.02	0.02	-	0.02	-	-	0.02	-	0.02	-	-	-	-	-	-	-
Xylene	-	-	-	-	-	-	-	-	-	-	-	0.13	-	0.13	-	-	1.23	1.23
Toluene	0.08	0.08	0.19	0.21	-	0.21	-	-	0.11	0.10	0.11	1.02	0.08	0.94	-	-	1.29	1.29
Triethylbenzene	-	1.23	1.79	1.86	1.86	-	1.30	0.56	-	-	0.56	-	-	-	-	-	-	-
n-Propyl benzene	-	-	0.04	0.07	0.04	0.04	-	0.04	-	0.04	0.04	0.04	-	0.04	-	-	0.04	0.04
1,1-diphenylethane	-	-	-	0.20	0.20	-	0.20	-	-	-	-	-	-	-	-	-	-	-
1,2-diphenylethane	-	-	-	0.07	0.07	-	0.07	-	-	-	-	-	-	-	-	-	-	-
Butyl benzenes	-	-	0.68	0.79	0.69	0.10	0.01	0.68	-	0.10	0.68	0.10	-	0.10	-	-	0.10	0.10
Heavies	-	-	-	0.20	0.20	-	0.20	-	-	-	-	-	-	-	-	-	-	-
Total	24.86	51.47	675.15	674.63	31.49	643.13	2.25	29.25	594.43	48.70	623.68	332.96	26.64	306.32	27.68	332.01	647.94	9913.52
Temperature inlet (°C)	79.72	280.80	270.05	270.05	373.71	241.50	406.58	371.24	237.09	304.91	242.01	308.55	79.72	135.36	270.33	224.04	141.00	102.84
Pressure inlet (bar)	1	50	50	50	25	25	25	25	25	25	50	25	1	1	25	25	1.2	1.2

Table 6. Styrene material balance 3.

Species	Stream Flow (kmol/h)														
	B37	B38	B39	B40	B41	B42	B43	B44	B45	B46	B47	B48	B49	B50	B51
Ethanol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Benzene	4.64	6.59	0.00	-	0.34	7.18	1.01	6.17	-	6.17	-	-	6.17	6.17	0.00
Water	9263.26	9262.04	9234.77	9265.58	5.53	21.75	9.76	11.99	-	11.99	-	11.05	0.93	0.93	-
Ethylbenzene	447.27	346.10	-	-	1.58	344.52	7.45	337.05	0.02	0.74	336.31	-	0.74	-	0.74
Diethylbenzene	0.55	0.55	-	-	0.00	0.58	-	-	0.58	-	-	-	-	-	-
Styrene	180.04	272.66	-	-	0.82	271.83	0.05	3.85	267.93	0.00	3.85	-	0.00	-	0.00
Glycerol	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Hydrogen	209.53	319.68	0.00	-	319.46	0.22	0.22	0.00	-	0.00	-	-	0.00	0.00	-
Carbon Dioxide	10.72	16.36	0.01	-	15.54	0.82	0.82	-	-	-	-	-	-	-	-
Ethylene	5.21	6.54	0.00	-	6.29	0.25	0.25	-	-	-	-	-	-	-	-
Methane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Xylene	1.23	1.13	-	-	0.00	1.25	0.02	1.10	0.13	0.00	1.10	-	0.00	-	0.00
Toluene	13.43	20.48	-	-	0.26	20.22	0.99	19.23	-	18.88	0.35	-	18.88	0.18	18.71
Triethylbenzene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
n-Propyl benzene	0.04	0.04	-	-	0.00	0.04	-	-	0.04	-	-	-	-	-	-
1,1-diphenylethane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1,2-diphenylethane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Butyl benzenes	0.10	0.10	-	-	0.00	0.10	-	-	0.10	-	-	-	-	-	-
Heavies	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	10,136.25	10,252.51	9234.78	9265.58	349.82	668.96	20.00	379.40	269.57	37.78	341.62	11.05	26.72	7.28	19.45
Temperature inlet (°C)	102.84	516.00	40	30	30.000	30	30	41.27	41.27	69.44	147.96	30.00	30.00	30.00	48.08
Pressure inlet (bar)	1.2	2.7	1.2	1.2	1.2	1.2	1.2	0.1	0.1	1.2	1.38	1.2	1.2	1.2	1.2

5. Feasibility Analysis

5.1. Environmental Sustainability and Life Cycle Assessment (LCA)

Ensuring environmental sustainability in the design and operation of the styrene plant is paramount to the long-term success of the project and necessitates innovative technologies to minimise ecological impact.

5.1.1. Land Emissions

The plant will use up a higher-than-average area of land to safely store the reactors, which counts as land emissions, as they could be built on top of local habitats or require sea pipes that affect coastal marine life, wherein many ecologically important areas of coral reefs, mangroves, and migrating bird sites are protected by law and cannot be built upon [61]. There are three main layers of regulation to protect endangered habitats. The Coastal Regulation Zone (CRZ) limits development within 500 m of coastal areas. The Environmental Clearance under EIA notification, 2006, dictates a biodiversity management plan and an environmental impact assessment (EIA) [62]. Finally, Wildlife Protection and eco-sensitive zone clearance are also necessary if the plant is located within 10 km of any national park and requires additional clearances, which demonstrate there is no net loss of critical habitat. Before the plant site is built, a Coastal Ecologist is required to map any important boundaries close to the site, then an NBWL-approved document is required to complete the wildlife clearance documentation and approvals, which can take 3–6 months.

There will also be additional traffic caused by heavy vehicles for the construction of the plant. To collect the 532,000 tonnes of corn stover per annum, a trucking system could be used; however, it would require around 8 truckloads of corn stover per day, much lower than that of large-scale plants [63–65]. Alternatively, transportation pipelines from surrounding farms could be used if strong relationships with farmers are developed. There is the potential for saccharification to happen if the pipe could be heated economically as it travels to the plant and reduce the number of reactors and their cost. However, a minimum 20%-solids pipeline system could be used. Alternatively, there is the potential for local ports to ship in corn stover from other parts of India; however, this is unlikely to be cost-effective, and so every effort should be made to create ethical relationships with local farms to buy in corn stover and develop appropriate pipelines in accordance with local community planning. The pipelines should be checked regularly for leaks to avoid waste, even if non-hazardous. The use of pipelines could also limit the initial corn stover storage requirements.

From the bioethanol section of the plant, there will be some solid waste in the form of lignin, hemicellulose, and cellulose. This can be sold as a feedstock, for example, as bioadhesives. If, due to market saturation, it cannot be sold or given away, it can be combusted in a boiler in line with the Air (P&C) Act stack emissions limits for biomass boilers or used as compost. The latter two are to be avoided at all costs, as this would add significant emissions to the plant. The remaining lignin, cellulose, and hemicellulose sludge in water from the dryer would be classified as non-hazardous organic sludge. Presuming it is beneath the HWM Rules thresholds, it can be managed under the Solid Waste Management Rules, 2016 [66]. This means it can either be dried further as far as economically feasible, or anaerobically digested to produce biogas, with the remaining effluent discharged once in line with the Water (P&CP) Act and Environment (Protection) Rules and CPCB Effluent Standards, for which the Environment (Protection) Rules (1986) state that less than 100 mg/L is acceptable. Alternatively, for minimum processing, it can be spread as a fertiliser material once assessed for heavy metals under the Fertiliser Control Order.

If it is uneconomical for the above to take place onsite, especially due to size limitations, or in the case of emergency shutdowns or plant damage, offsite treatment of the waste stream can take place. Spent hazardous materials are transported via GPCB-compliant (Gujarat Pollution Control Board) transport to one of the registered and authorised TSDFs (Treatment, Storage and Disposal Facilities), as there are several located in Gujarat [67]. Alternatively, if non-hazardous, as suitably evaluated under the Bureau of Indian Standards 9040 C guidelines [68], they may go for composting at the facility.

The site should also have annual third-party verification audits to check for leaks before they become significant enough to be violations. Soil runoff potential from leaks or spills can be prevented with internal EMS audits and annual environmental compliance audits, as laid out in the CPCB (Central Pollution Control Board) guidelines. There should be regular monitoring of installed wells downgradient of any storage areas, or monthly during rainy seasons. Soil sampling should also take place both onsite and in surrounding areas, in the topsoil and subsoil (down to 1 m) annually, for VOCs, heavy metals and pH [69]. Soil-gas monitoring should also take place, as vapour emissions of harmful substances caused by leaks will collect underground. These should be monitored continuously with PID sensors or monthly with GC sampling for VOCs, BTEX and aromatics. Leachate and stormwater surveillance can also function as an indicator of leaks, as well as ground emissions.

5.1.2. Air Emissions

In the continuous section of the plant, there are three main air emission potential streams: 25, 41 and 43, stream 41 is 91% hydrogen, which has, in total, been produced from corn stover, so it could count as partially carbon neutral. The stream also contains trace amounts of ethylene, benzene, water, ethylbenzene, carbon dioxide toluene styrene, diethylbenzene, xylene, propyl benzene, and butylbenzenes. Stream 25 contains mostly diethylbenzene, and stream 43 contains mostly water and ethylbenzene. Due to the nature of the VOCs in the stream and their potential as carcinogens to humans, they must not be directly released in any amounts and must be converted to safer compounds. Since parts of the plant cannot be heated by heat exchanger steam due to temperature difference considerations, this stream is used as fuel to minimise the amount of mined natural gas that would otherwise be required. When hydrogen combusts, it only creates water vapour; hydrocarbons will produce CO₂, or CO in improper combustion. There is also the risk of generating thermal NO_x at elevated temperatures, which is a key driver of ground-level ozone depletion and photochemical smog.

The Prevention and Control of Pollution Act of 1981 and the Environmental Protection Act of 1986 set out regulations in India regarding air pollution, set by the CPCB. Furthermore, the Hazardous Waste—Management, Handling and Transboundary Movement—Rules, set in 2008, require that such waste streams obtain authorisation from the State Pollution Control Board (SPCB) before the operation of the plant begins, and, more specifically, the Environmental Protection Fifth Amendment Rules of 2008, lay out the requirements related to emissions of common hazardous waste incinerators [70]. These guidelines are the specific standards for safe incinerator design. Most importantly, there is the requirement for twin-chamber incinerators with a minimum temperature of 950 °C and a residence time of over 2 s. To ensure total combustion of carcinogenic compounds, the CO₂ present in tail gases must be over 7% (O₂ corrected). To maintain a high standard of burn, a continuous emission monitoring system must also be installed per CPCB's 2018 guidelines, which describe different options of monitoring and the most up-to-date emission limits, as shown in Table 7 [71].

Table 7. Common hazardous waste incinerator emissions limits [69].

Species	Limiting Concentration mg/Nm ³	Sampling Duration mins
Particulate Matter	50	30
HCL	50	30
SO₂	200	30
CO	100	30
	50	24 (h)
Total Organic Carbon	20	30
HF	4	30
NO_x	400	30
Total dioxins and furans	0.1 ngETQ/Nm ³	8 (h)
Cd, Th, and related compounds	0.05	2 (h)
Hg and compounds	0.05	2 (h)
Sb, As, Pb, Co, Cr, Cu, Mn, Ni, V, and compounds	0.5	2 (h)

It is also unlikely that VOCs would be stored for a long time. However, in cases of emergency shutdown, the tanks that house the reactor output must be fixed-roof tanks that use vapour recovery to the incinerators. This legislation suggests the need for backup incinerators if the main ones are not operational, which can achieve over 99.9% VOC removal. Furthermore, a Leak Detection and Repair programme is required to check all pumps, valves and flanges that manage hydrocarbons quarterly to minimise leakages, as well as to address any visible leaks and replace components [47].

With a well-optimised process for incineration, the main emission from the gas stream is carbon dioxide, which ideally should be captured. Although many technologies are still in their infancy, chemical absorption from amine scrubbing could remove some CO₂ if it were to be cost-effective to do so, with some estimates placing it at \$50–75/ton to remove. Alternatively, because the outlet is mostly steam otherwise, the CO₂ could be separated off and sold for carbonated beverages or ammonia synthesis. It should be noted here that the final product is partially carbon neutral due to sourcing from corn stover; more work could be done to find lower-carbon benzene sourcing when economic routes become available and in capturing the final emissions from fuel and waste incineration, which would further decrease the overall emissions of the plant [72].

5.1.3. Water Emissions

After steam has been recycled for heat integration purposes, it is used as water, as well as a sea cooling system for the largest heat exchanger. The outlet of the exchanger must be no more than 7 °C higher than the inlet temperature, as designated by the Environmental Protection Rules of 1968, Section 84 [47]. This will have seasonal variations, so the heat exchanger has been designed with the average in mind. The water also needs to be checked for released contaminants, as, in line with the Environmental Protection Rules of 1986, it should be monitored for pH levels, oil, and grease, and they should not exceed 1 mg/L. The former is also bound by concentration limits; the current mass balance shows all water output contains 0.0001 kmol/h benzene at most in 9234 kmol/h of water, which is a concentration of 0.052 mg/L; even with the reduced steam from the PBR optimisation of 5000 kmol/h, it would still be beneath the limit at 0.095 mg/L. Similarly to air emissions,

this would require regular monitoring to ensure it is meeting the regulatory requirements. Furthermore, any oil separators or equalisation tanks need floating or fixed covers to remove gases (such as styrene from stream 45), which can then be added to the gas emissions stream and dealt with as above. Any streams that are found to contain trace amounts of benzene or xylene must also be treated to a level of 10, 20 ppm respectively, which would only happen if there was a serious fault on a piece of manufacturing equipment and could be detected by the analysis transmitters on the P&ID [47].

There is a sodium hydroxide waste stream; however, this is recycled through the chromatography column. This process cannot be completely effective, so any outlet stream must be pH-checked for trace amounts and, if necessary, neutralised, as set out within the Hazardous and Other Wastes (M&H) rules 2016 [73]. Hydrogen Chloride is also considered a hazardous material and dealt with under these guidelines, as an acid using caustic soda (NaOH) if required or sent for treatment at an appropriate TSDF.

Sodium carbonate in water is considered a non-hazardous alkaline effluent and can be crystallised for reuse with a pH adjustment; however, if trace amounts are released, they must be under 30 mg/L as per the Water (P&CP) Act, 1974 and the Environment Protection Rules, 1986, to meet the effluent norms.

5.1.4. Life Cycle Assessment (LCA)

The Life Cycle Assessment (LCA) is the most practical numerical evaluation tool that can assess the carbon emissions and other impacts on the environment throughout the system and functional life of the plant. There are many data limitations in doing this, so we assume a cradle-to-gate or gate-to-gate approach. What happens after the styrene and side products are sold will depend on their use as hard or soft plastics, building insulation, tyres, or adhesives, each of which will have different end-of-life options and destinations. The gate-to-gate approach, where only the emissions relating to the plant are considered, exclusive of initial transport costs and end-of-life uses, is therefore chosen. As shown in the boundary diagram below (Figure 4), the simplified plant with its environmental inlets and outlets can be used for evaluation.

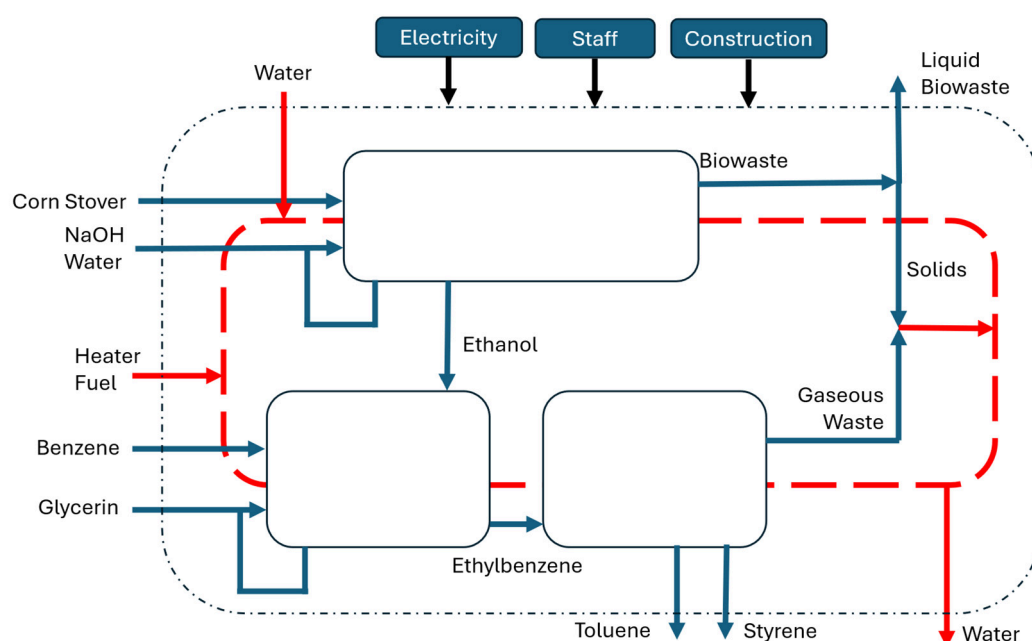


Figure 4. Functional unit being analysed showing system boundaries, and the total inputs and outputs of the system.

Firstly, there are ways plant manufacturing emissions can be minimised, such as building on currently designed plants or repurposing previous sites to prevent excess habitat loss. Construction vehicles and lorries have the potential to be electric or hydrogen-based; however, charging points are harder to access in rural India than in areas of the UK. The metals for the reactors and tanks could come from mined or recycled sources; however, the purity of the steel is paramount to preventing corrosion and containing stresses, and so recycled metal could come with problematic impurities and would need to be checked carefully. Finally, concrete creates large emissions, which can be reduced by up to 45% by capturing the carbon resulting from the limestone pre-calcination process, or other types of concrete carbon-capturing technology [74].

Once the plant is functional, the main lifecycle considerations are the inputs and outputs. The waste streams are mostly integrated into the system because, due to the required furnace heat, an electric heater cannot be used. Therefore, to minimise emissions, the waste streams are burnt onsite to generate energy. These streams are mostly hydrogen formed from the ethylbenzene, which is 50% from renewable corn stover and 50% from benzene (the latter having no renewable producers). This is then integrated into the furnace system to heat the required streams. The toluene and styrene are sold off, while the wastewater is treated and recycled back into the system, eventually being treated and released. The liquid bio-waste is also sent off to be used in agriculture.

To estimate data for the lifecycle of the plant, the CCaCL2 programme was used, which was purpose-created by the University of Manchester [75]. To accurately estimate this, the plant was modelled as a single system to consider the overall inputs and outputs of chemicals and energy. No emissions for packaging were included, as the chemicals would be stored in tankers for transportation or in tanks onsite. Glycerine and sodium hydroxide were added on the basis that, although recycled, they would still need regeneration every 2 years, and thus the emissions should be considered. Water was added from a ground-water source in India, instead of the standard option for plant water, to account for water scarcity issues. Benzene and corn stover were added as normal chemicals. The system energy was also added to be as close as reasonably possible to the real design, given the system limitations.

The process-related environmental emissions were allocated using an economic allocation approach, reflecting the relative market values of the products. As styrene is the primary value-added product, it is estimated to account for approximately 95% of the total plant revenue. Consequently, 95% of the total environmental emissions were allocated to styrene production, while the remaining 5% were attributed to the recovery of by-products. This allocation highlights the environmental benefit of by-product valorisation, demonstrating that the recovery of secondary products incurs only a small proportion of the overall environmental burden while contributing to improved resource efficiency and process sustainability.

As shown in Figure 5, the life cycle assessment (LCA) estimates that the proposed plant emits approximately 4000 kg CO₂-eq per operating hour, which is adopted as the functional unit for the assessment. Based on a styrene production rate of 27,794 kg h⁻¹, this corresponds to 0.143 kg CO₂-eq per kilogram of styrene produced for the assessed life cycle stage.

For comparison, conventional styrene production from benzene and natural gas is reported to generate approximately 2 kg CO₂-eq per kilogram of styrene, representing an environmental burden that is more than an order of magnitude higher than that of the proposed process [76]. The substantial reduction in greenhouse gas emissions is primarily attributed to the rigorous heat integration strategy implemented throughout the plant, which significantly reduces the external energy demand and the associated emissions from fuel combustion.

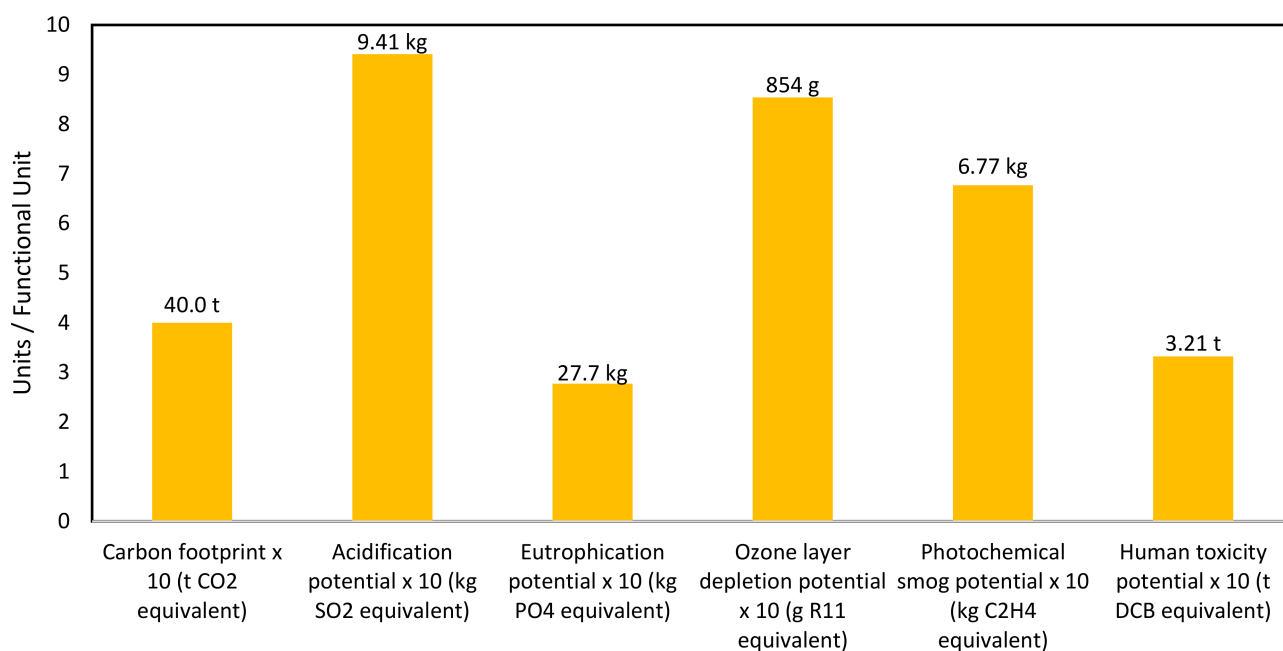


Figure 5. Multiple impact graph [75].

Furthermore, the process enhances resource efficiency by utilising the hydrogen generated during ethylbenzene dehydrogenation, together with waste streams from the bioethanol production process, as supplementary combustion fuels, thereby reducing reliance on fossil energy sources. The combustion of residual corn stover-derived biomass is considered effectively carbon neutral, further lowering the overall carbon footprint. In addition, the carbon dioxide generated during fermentation is captured and recycled for use in the lignin precipitation stage, as described previously, further improving carbon utilisation and the overall sustainability of the proposed process.

The proposed process also exhibits a relatively high water footprint, primarily due to the substantial steam demand in the packed-bed reactors, water requirements for the fermentation process, and the extensive heat integration network. However, a significant proportion of the process water can be recycled and reused multiple times before replacement, subject to acceptable contaminant levels. The implementation of appropriate water treatment and contaminant removal technologies would enable extensive water recirculation, thereby substantially reducing freshwater consumption. Such an approach would not only improve the overall sustainability of the process but also minimise potential pressures on local water resources, particularly during periods of seasonal water scarcity.

The ozone emissions for the process are 8.54 gR11 equivalent per 27,794 kg styrene, which is 3.07×10^{-7} kgCFC-11 equivalent per 1 kg of styrene. Normally, the ozone depletion of styrene production is somewhere between 2×10^{-7} and 4×10^{-7} kg CFC-11 equivalent; however, this is still higher than the LCA from the conventional process, which was 1.86×10^{-15} kg CFC-11 eq [76]. This is mostly due to the addition of solar panels, which the software counts as 1.867×10^{-5} kg R11 equivalent/MJ, which is far higher per MJ than natural gas (1.518×10^{-10} kg R11 equivalent/MJ) and hydrogen.

5.2. Economic Evaluation

The prices are calculated based on the 2025 price index. However, the plant will be allowed approximately 3 years to build. Therefore, the year in which the plant will be fully ready to operate and generate profits is set to be 2030 as the first year with internal free cash flow. The price indices used are given below (Table 8):

Table 8. Price index [77].

Year	Price Index
2004	143.7
2025	293.9

The economic analysis comprises the estimation of the initial capital investment, net future worth (NFW), payback period, net present worth (NPW), rate of return (ROR), and discounted cash flow rate of return (DCFRROR). The analysis begins with the determination of both capital and operating costs using a detailed factorial cost estimation approach.

Equipment purchase costs were estimated using the cost correlations together with current land costs for the proposed plant location in Gujarat, India [78]. The purchase costs, originally based on mid-2004 values, were updated to 2025 prices using the appropriate cost escalation indices to reflect current market conditions. Table 8 summarises the estimated purchase costs for the major process equipment and the corresponding total capital investment, while the final fixed capital cost estimates are presented in Table 9.

Table 9. Capital costs of the plant.

Capital Costs						
Equipment List	Quantity	Size Range	Constant	Index	Cost per Unit	Total Cost
Pumps	11	250	2700	0.8	223,726	2,460,982
PBRs	4	30	1500	0.4	5847	23,388
Compressors	16	100	1920	0.8	76,437	1,222,985
Furnaces	4	1000	560	0.77	114,337	457,349
Decanters	2	5000	100	0.8	91,028	182,056
Evaporators	2	50	10,000	0.52	76,465	152,931
Mixer	2	30	1900	0.5	10,407	20,813
Crusher	3	100	3800	0.85	190,451	571,353
Batch reactor	2	30	15,000	0.4	58,471	116,942
Separator	4	0.8	5800	1	4640	18,560
Filter	2	25	8800	0.6	60,708	121,416
Washer	1	20	1900	0.5	8497	8497
Dryer	2	5	7700	0.35	13,525	27,050
Tanks	19	50	2400	0.6	25,095	476,812
Reboiler	13	25,000	120	0.8	395,852	5,146,081
Condenser	13	300	1920	0.8	184,076	2,392,994
Heat Exchangers (HX)	18				20,000	360,000
Cooling tower	1					100,000
Distillation Columns	13					1,040,000
Ex-TSSF cost total						14,900,210
Equipment cost (Post TPSSF)						21,000,000
Total reactor cost (ex lang factor)						35,900,210

Table 9. Cont.

Capital Costs						
Equipment List	Quantity	Size Range	Constant	Index	Cost per Unit	Total Cost
Total Cost (Post Lang Factor of 3.6) (ex-inflation adjustment)						129,240,756
Total cost (post adjustment) (2025) (ex-land price)						264,327,474
Cost of land						945,654
Total cost (post adjustment) (2025) (post land price)						265,273,128

Following the estimation of the fixed capital investment, the annual operating costs were determined based on the methodology and assumptions summarised in Table 10. The cost of corn stover was assumed to be \$71 per tonne, which is a consistent value among the literature [79,80]. The costs of the remaining raw materials and utilities were estimated using the cost correlations and economic data commonly used in plant design [78]. These operating cost estimates form the basis for the subsequent economic evaluation of the proposed process.

Table 10. Operating costs of the plant.

Operating Costs		
Operating Costs	Subtotals	Total Cost per Input
Raw Materials		169,965,472
Benzene	147,020,424	
Corn stover	19,715,216	
Catalyst (PBR)	1,508,107	
Catalyst (Bioreactor)	969,505	
Water	752,220	
Utilities		42,082,969
Laboratory Costs		201,600
Maintenance		26,432,747
Plant Overheads		2,643,275
Operating Labour		1,008,000
Capital Charges, Insurance		26,432,747
Indirect production cost		53,753,362
Total		322,520,173

The economic potential of the plant has been examined over the 25 years from 2025 to 2050, based on the revenue generated, cash inflows and outflows, inflation rates, taxes, and depreciation to determine the net present worth and discounted cash flow of the plant. The plant has been allowed the first 3-year period, starting from 2025, to be built and is therefore expected to start operating to generate revenue from 2028 as the first year.

The revenue generation from the four products: styrene, toluene, animal feed, and bioethanol remains consistent throughout the forecast period, with the major revenue contribution coming from styrene, valued at approximately \$378.4 million annually. Other materials, such as toluene and animal feed, contribute much smaller but steady amounts

of around \$18.13 million and \$3.41 million per year, respectively. However, the styrene production capacity will not be reached in the very first year of operation. Therefore, the revenue generated from the products would be lower than expected but progressively increasing towards reaching the target capacity. Once the plant reaches the target, it then continues generating 220,000 tonnes per year over the 25 years of the forecast.

The selling price of these materials drives a total annual revenue of approximately \$400 million, which is subject to change over the years, but in this case, it is assumed to remain stable throughout the forecast period, indicating predictable revenue generation and market stability.

During the first few years of plant building and design, there will be no operating costs involved, as the plant will not be ready to operate and produce styrene yet, so it will only be using the initial investment, also known as the total fixed capital cost, to build the plant. Then, after it is built, the operating costs become involved, and the plant starts producing styrene and hence revenue. But there will be no profit even though there is cash flow within the plant, due to the plant still paying back its initial capital costs while it was being built and not generating any revenue. Therefore, the net profit is negative, as illustrated in the graph shown in Figure 6.

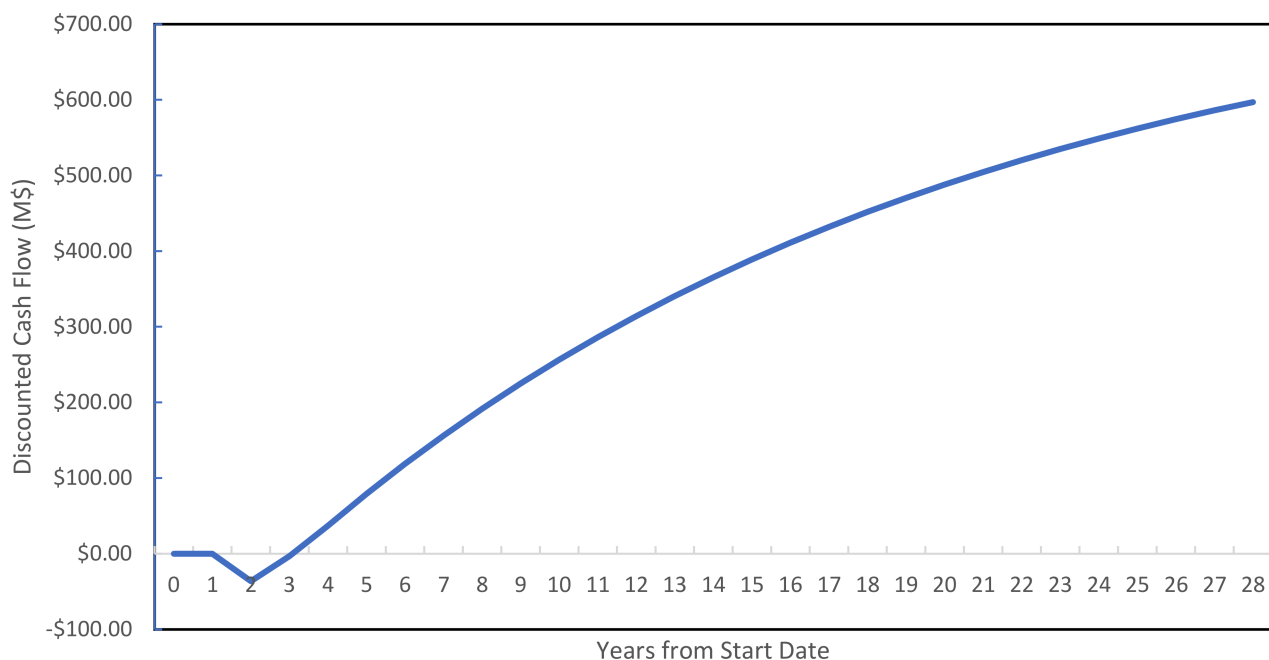


Figure 6. Cumulative Discounted Cash Flow.

The operating costs are calculated to be \$322.5 million each year; however, they are likely to vary depending on how much maintenance the plant requires over time to fix or replace faulty equipment. But if the operating cost is taken to be consistent, then it would indicate operational efficiency and stable production costs. This assumed consistency, combined with stable revenues, implies that the business can operate with high cost predictability and financial stability.

The operating costs begin to rise near the end of the forecast period due to an increase in the maintenance costs for the wear and tear of the plant equipment. This is demonstrated by the slight decrease in gradient towards the end, at the top right of the graph below (Figure 6). This increase in maintenance costs leads to a decrease in profit margin near the end of the project lifespan, as the plant is using more money to maintain the production capacity and keep generating revenue.

Figure 6 also shows how the profit starts to increase after a few years of operation as the plant begins to generate more profit. The payback period can be seen as well, where the plant completely recovers the initial investment, which is about 6 years, including 3 years of building and 3 years of operation. The point where the line crosses the x-axis while moving upwards is the break-even point, and that is the point where profit earned is technically zero because all the money is used to pay back the initial investment.

Earnings before interest, taxes and depreciation stand at about \$86.7 million per year, representing a 21.2% profit margin on total revenues. The high margin indicates that the business maintains a strong operational performance, ensuring substantial profitability even as revenues and costs remain steady. This margin is a key indicator of the plant's ability to manage operational costs effectively while maximising its output.

The plant has a tax rate of 35%, which is specific to the location of the plant in Gujarat, India. The plant generates an estimated net profit after tax of around \$45.7 million annually, reflecting a steady after-tax profit during its peak years of operation. This indicates the plant's strong ability to convert operating profits into net profits, suggesting a sustainable and healthy business model with ample room for reinvestment.

The net cash flow provides a clear and intuitive measure of profitability by representing the difference between the cash inflows generated by the project and the cash outflows required for its operation. It also forms the basis for several more advanced economic performance metrics, such as Net Present Worth (NPW), Internal Rate of Return (IRR), and payback period. While the cash flow figures initially provide a straightforward view of profitability, further refinement would be essential to reflect real-world economic impacts, particularly taxation and depreciation. In many industrial economic analyses, tax and depreciation are either simplified or omitted in early calculations due to variations in local tax codes and accounting standards. However, for a more realistic projection, corporate income tax, which is typically between 25 and 35% in India, has been included in profit estimates, as it significantly affects the net earnings. Depreciation also plays a crucial role as it reduces the taxable income over the useful life of assets, particularly when accelerated depreciation schemes or capital grants are provided by government policies to encourage investment. A more refined financial assessment involves accounting for the time value of money using discounted cash flow (DCF) techniques, as demonstrated in Figure 7. This recognises that money earned earlier in the life of a project has greater value than money earned later, as earlier revenues can be reinvested to generate additional returns. Each year's cash flow is therefore discounted to its present value using a selected interest or discount rate, providing a cumulative figure known as the Net Present Worth (NPW). In this case, the discount rate has been taken from the bank borrowing rate in Gujarat, India, which is currently 6%. A project with a positive NPW at a realistic discount rate is financially viable. Another related measure is the discounted cash flow rate of return (DCFRR), which is the interest rate that brings the NPW to zero and serves as a robust indicator of a project's long-term profitability.

In addition to NPW and IRR, the payback period offers a practical perspective by indicating how quickly the initial capital investment is recovered through project income. While commonly used for short-term projects or incremental plant upgrades, the payback period does not account for cash flow beyond the recovery point and therefore may overlook long-term profitability. Furthermore, inflation, a critical macroeconomic factor, must be acknowledged, as it erodes purchasing power over time. In economic projections, inflation can be incorporated either by adjusting the discount rate or by applying separate inflation factors to revenues, operating costs, and raw material prices, recognising that each cost component may be affected differently.

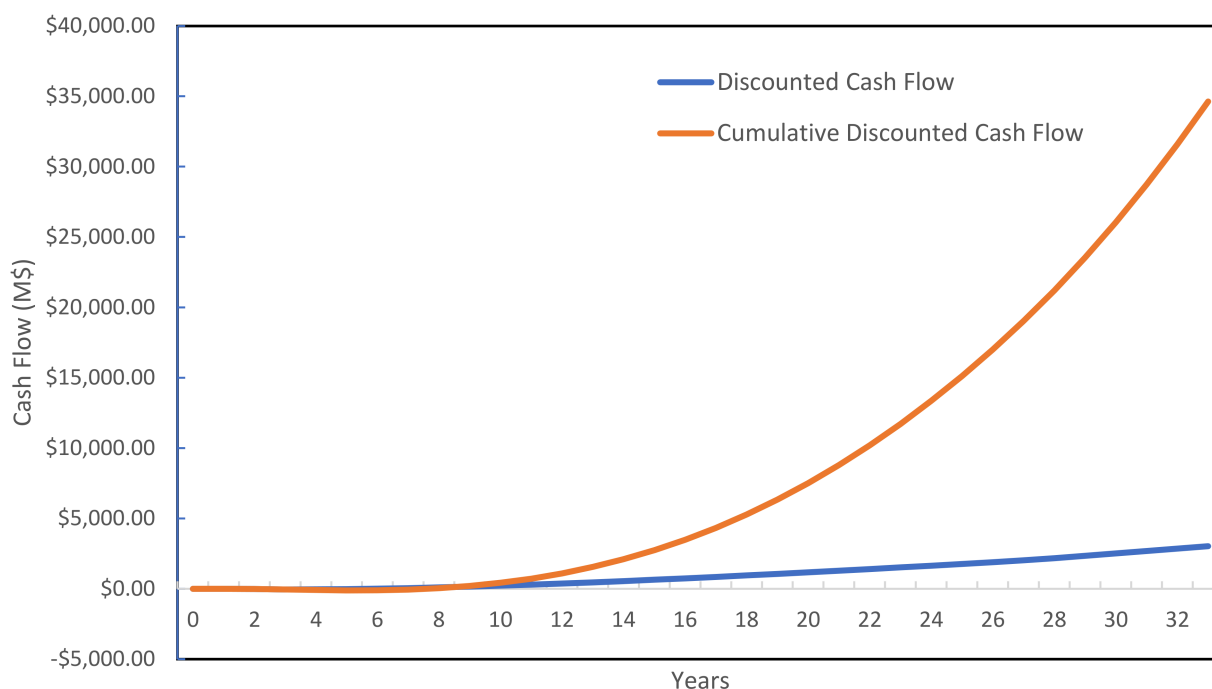


Figure 7. Cumulative Graph of Discounted Cash Flow.

Furthermore, a project's Rate of Return (ROR) provides a simplified, yet valuable snapshot of how effectively the invested capital is being utilised. While ROR is typically calculated based on average annual profits and the original capital investment, its simplicity may obscure variations in cash flow and overlook the time value of money. Therefore, in rigorous evaluations, ROR is best used in conjunction with more dynamic measures such as IRR and NPV. Overall, the economic viability of the styrene production facility depends not only on achieving strong annual cash flows but also on how those earnings are evaluated within the broader financial framework, including taxation, depreciation, discounting, inflation, and capital recovery.

The Free Cash Flow (FCF) or Net Cash Flow is derived by adding depreciation to the net operating profit after tax, with no significant changes in working capital or capital expenditures projected. As a result, the plant generates an estimated FCF of \$265 million during its peak years of operation. This consistent free cash flow is an indicator of the plant's capacity to generate cash to cover any future operational needs, debt servicing, and dividend payouts, which will be crucial for sustaining long-term growth and stability.

The discounted cash flow (DCF) is calculated using a discount factor that accounts for the time value of money. Over the past 25 years, the plant's future cash flows have been discounted to provide a more accurate representation of its current value. The discount rate is increased by a compound formula every year. For this plant, the IRR was calculated to be 28% as a percentage, which is favourable, with a total NPV of \$183 million USD for the 25 years. The return on investment (ROI) is 17.2%, which is a reasonable percentage of return on the investment made. These are estimates made based on how the plant is expected to run during the forecast period but are subject to varying conditions depending on the market rate and the economy of India over these years of operation.

The proposed process demonstrates strong economic performance, comparing favourably with conventional styrene production, which has been reported to achieve a net present value (NPV) of approximately \$105 million. The enhanced economic viability of the proposed design is reflected in its higher NPV and internal rate of return (IRR), primarily attributable to extensive material integration, rigorous heat integration, efficient by-product recovery, and reduced operating costs [81,82].

These economic indicators demonstrate the strong financial viability of the proposed plant and establish a solid foundation for long-term commercial success. The favourable net present value (NPV), internal rate of return (IRR), return on investment (ROI), and stable cash flow indicate that the project is capable of generating sustained value for investors throughout the project lifetime. Furthermore, the projected stability of key economic parameters, including revenue, operating costs, and cash flow, supports the long-term profitability and resilience of the proposed process, as illustrated in Figure 8.

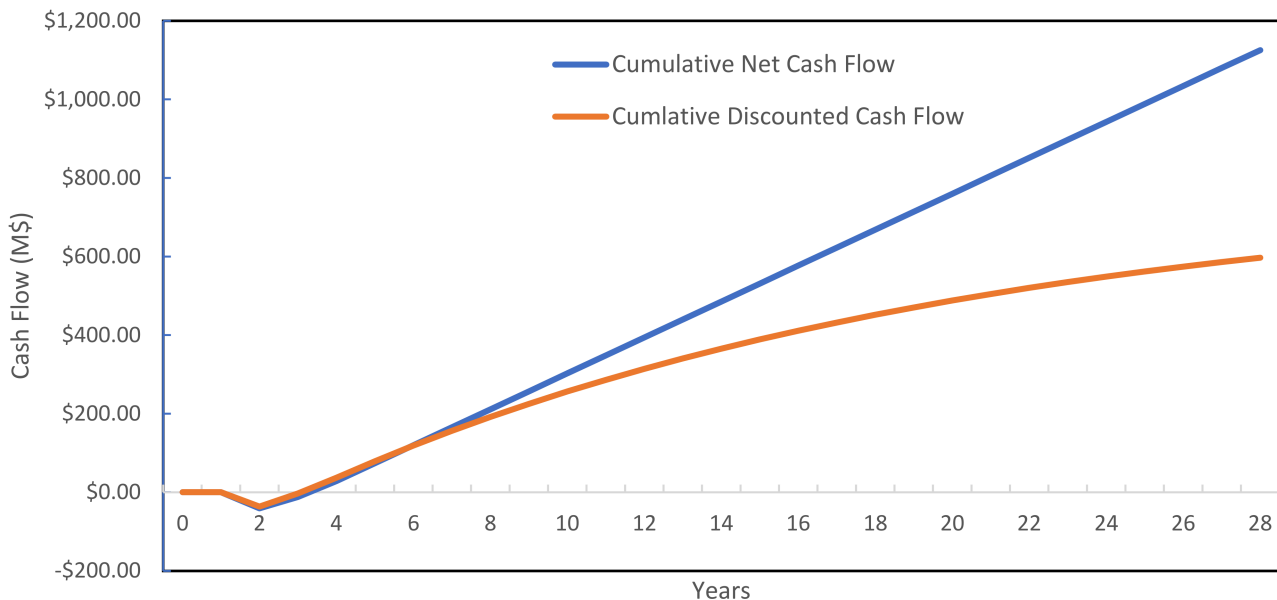


Figure 8. Cumulative Graph of Net Cash Flow vs. Discounted.

5.3. Social Impact

Ethics are a priority to ensure the styrene plant brings tangible benefits to the local community. Employment opportunities would be created for the local population through targeted local hiring and training programmes designed to develop necessary skills. Robust health and safety protocols are paramount to protect both workers and surrounding communities, including measures for the safe handling of hazardous materials and emissions control that go beyond the law, as well as the establishment of emergency response plans [83]. Transparent communication channels should be established with local stakeholders to address potential concerns. Furthermore, the project would contribute to community development by investing in essential infrastructure such as schools, healthcare facilities, and access to clean water, alongside supporting local businesses and fostering mutually beneficial partnerships. India, which has often had a monopoly on the engineering sector, produces around 1.5 million engineers annually. In recent years, the employability of these engineers has been a major issue, as there are too many engineers for the number of jobs available, with reports suggesting that only 10% of graduate engineers will secure employment, leading to an abundance of available engineers [84]. The building of a plant of this scale in the industrial powerhouse of Gujarat, India, would contribute to reducing unemployment rates. India also has a similar government policy encouraging self-manufacturing and making dedicated investments into manufacturing with “Make in India,” which was launched in 2014 [85].

6. Risk Assessment/Mitigation

6.1. Process Safety—HAZOP

Safety is the most important consideration for a chemical plant, as before a plant can be profitable, it must be safe to operate. Strict standards are in place in both the UK and India regarding the protection of workers, residents, and the environment. Continuous audits are done throughout the life of the plant on its operational state and practices to ensure its standards are being upheld. The Health and Safety at Work Act of 1974 is the most fundamental legislation for workplace safety in the UK, with the equivalent act in India being the Factories Act 1948 (amended 1987). There is also the British standard ISO 45001 [86], which deals with occupational health and safety, and ISO 12100 [87], which covers risk assessment and risk reduction for machinery. Meanwhile, in India, BIS IS 15656 risk assessment codes, as well as the occupational safety, health and working conditions codes of 2020, will also apply. There are also strict chemical safety regulations in both countries, which will apply to the handling, storage, and emissions of hazardous chemicals. The Control of Major Accident Hazards (COMAH) Regulations of 2015 in the UK set out the requirements for safety reporting, emergency planning, and public information. The Indian equivalent is the Manufacture, Storage, and Import of Hazardous Chemicals Rules, 1989 (MSIHC Rules).

A Hazards and Operations Study (HAZOP) is a process that identifies potential hazards in a chemical process before they can cause incidents. It is conducted as a group through a series of meetings that analyse a chemical plant section by section. Specifically, the HAZOP regulations in the UK are set out in the HSE guidance HSG 190, which gives the best practices to use when conducting a HAZOP. The closest Indian equivalent is set out by the Oil Industry Safety Directorate (OSID) guidelines for process safety and HAZOP.

HAZOP has a specified process, whereby the plant is broken down into nodes, usually individual components or fewer, and a guideword such as MORE, LESS, REVERSE is applied to a process parameter such as FLOW, TEMPERATURE, PRESSURE, etc., and what could become a hazard for each combination of guideword and parameter is assessed for possible consequences, existing safeguards and recommendations for avoidance. Finally, this is recorded line by line with risks and actions in a HAZOP table. Table 11 shows the HAZOP process for a batch reactor in the bioethanol process.

Table 11. HAZOP table for STR1.

Item	Study Node	Process Parameter	Deviations	Potential Causes	Possible Consequences	Current Safeguards	Action Required
STR1	Batch reactor	Flow	NO, NOT, NONE	Valve malfunction, blockage of product due to lack of water, or a leaky valve	Spillage of product, loss of money, no reaction, time wasted, extra storage needed while repairs happen, loss of income		Flowmeter on inlet valve sending details to the control room, regular checks on valves before each/every 10 batches
			NO, NOT, NONE	NaOH tank valve malfunction	Reaction does not proceed and needs additional cycles, loss of money, time wasted, and further issues down the line if not realised	pH testing system	Sample analysis to check the reaction has gone through and avoid quality issues
			MORE, GREATER, HIGHER	Valve stuck open/opened, higher flow rate than intended	Overfilling of batch reactor, leakages or overpressure, acid or pH issues	Level flow to open the exit valve	Flowmeter on inlet valve, fail-closed valve to prevent overfilling if valve has issues
			REVERSE	Overfilled batch reactor	Corn stover going back to the tank, time and money wasted, equipment damage, or NaOH going out of the designated system	pH testing system	Stop-check valves on the NaOH and water, and the inlet valve

Table 11. Cont.

Item	Study Node	Process Parameter	Deviations	Potential Causes	Possible Consequences	Current Safeguards	Action Required
		Temperature	NO, NOT, NONE	Winter conditions (low outside temperature) and lack of extra heating	Slower reaction, time, and money wasted, incomplete reaction when released	Temperature checker	Availability of heat streams
			MORE, GREATER, HIGHER	The reaction goes too fast	Pressure increases or, if above a certain point, warping of the shell, extra side reactions or enzyme breakdown, and loss of money	Temperature checker, but not connected to anything	Check that steel and enzyme rates are suitable for the highest summer temperatures, and if not, add a cooling/heating combo jacket for year-round temp control
		Level	MORE, GREATER, HIGHER	Flow rate inlet valve malfunction or output valve malfunction	Overflowing of the batch reactor or overpressure, loss of money, degradation of enzymes if the wrong pH is reached; more money lost	Level metre to open at the bottom with fail-open valve	Connect the level metre to the flow inlet valve
			LESS, LOWER	Flowrate inlet valve malfunction or output valve malfunction	Underfilling of batch container, loss of money and profits, backlog of corn stover that needs processing, and extra storage costs	Level metre, alarm attached to valve	
		Pressure	MORE, GREATER, HIGHER	Inlet and outlet valve malfunction, heat of reaction getting too high, agitator working too hard	Explosion or damage to equipment, danger to life, loss of money and time	Fail-open valve	Pressure monitor and automated pressure relief valve going to a suitable-sized and graded tank for the pH
			LESS, LOWER	Lack of inlet flow rate or a sudden burst in the tank	Loss of product	Level metre	Pressure monitor linked to the inlet flow rate valve
		Concentration/pH	MORE, GREATER, HIGHER	Inlet valve from NaOH tank malfunction, or water valve malfunction	Issues later in the process as wrong pH impacts enzyme function, danger to human life if leaks occur, and money lost	pH metre	Flow rate metre on the valve or analysis transmitter to check, as well as a pH metre
			LESS, LOWER		Money lost, less product, and enzyme death		
		Agitation	MORE, GREATER, HIGHER	Overworking/malfunction of the agitator	Early end of life for the agitator, extra cost, enzymes accidentally destroyed, loss of profits from lower reaction rate		Regular tests and cleaning of the tank between batches
			LESS, LOWER	Fault in the agitator, something is getting stuck in the mechanism			
			SOONER THAN	Fault in the agitator or the control software	NaOH is being sprayed everywhere on workers, causing burns while doing maintenance. NaOH is being mixed around with no loss of product and extra cost in wasted materials		Regular testing and a velocity metre
			LATER THAN				
		Sample	NO, NOT, NONE	No/Fault in the analysis transmitter	Unable to tell if the reaction is working properly	Increases cost because it is hard to do an optimised reaction	Analysis transmitter, AIC, and analysis alarm to connect to the control room, with checks of sensors between batches
		Power	MORE, GREATER, HIGHER	Power surge	Explosion of electronics, failure of fuses or sensors, inability to control the plant, loss of money, danger to human life if chemical spills occur		Explosion-proof electronics and earthing lines to ground, backup generator
			NO, NOT, NONE	Lack of electricity, faulty wiring	Inability to control plant, lack of data, cost, danger to human life		Backup generator for plant if main does not work

6.2. Feedstock Supply Changing and Sourcing Strategies

The possibility of feedstock changes is unlikely to cause significant interference, as one of the main feedstocks is an agricultural waste product (corn stover), of which there will almost always be an abundance, while the other main feedstock is benzene, which India has been a high exporter of for many years, exporting 1.5 billion USD worth in 2024 alone [88]. In case of a benzene shortage in India, there are other countries in the vicinity, such as Thailand and Malaysia, which together export around 800 million USD worth of benzene, which should be enough to fuel our processes [88]. In the case of corn stover, while there is an abundance of it in India, due to poor/low harvests, corn stover might need to be supplied from elsewhere. In this case, China is the world's second-leading corn grower, producing 295 million tonnes per year, which exceeds the amount India produces, so it is a very dependable seller [25]. Additionally, if it is preferred to stay within India to save on importation charges, there is the option of switching temporarily to a different biomass, such as rice straw. While rice straw does have a lower percentage of cellulose and hemicellulose than corn stover, it is a very abundant agricultural waste, being the highest-yielding crop in India [89]. This is an attractive secondary sourcing strategy because the process of synthesising bioethanol from rice straw is remarkably similar to the process for corn stover, consisting of pretreatment, enzymatic hydrolysis, fermentation, and distillation [90].

6.3. Operational Complexity

As mentioned before, India currently has a very saturated engineering job market where many engineers are leaving university without the ability to get a job [84]. Additionally, the average wage for an engineer in India is 654,099 Indian Rupees (about \$7615 USD), which is significantly lower than the average wage of an engineer in a country such as the United States [91]. This value is also above the average wage for skilled workers in India, with an average of 546,000 INR (roughly \$6446.61). It is also important to consider that the cost of living and the cost of renting are both much lower than in countries such as the United States and the United Kingdom, which would call for a lower wage than in these countries. Gujarat, which is the state in India where the plant is assumed to be built, is well-known as the industrial heart of India, which is beneficial as it will be saturated with skilled workers to work at the plant [92]. Additionally, we can take advantage of the local Gujarat government policies that are further boosting industrial growth with policies that are providing land, tax incentives, and single-window clearance for industries starting up in Gujarat [93,94].

The principal engineering challenges associated with the proposed plant design are concentrated within the bioethanol production section, particularly in scaling up the simultaneous saccharification and fermentation (SSF) reactor from laboratory to industrial scale. Two critical factors govern successful scale-up: the high viscosity of the lignocellulosic slurry and the complex reaction kinetics associated with enzymatic hydrolysis and microbial fermentation.

The high solids loading required for economically viable bioethanol production results in a highly viscous slurry, which can significantly impair mixing efficiency and mass transfer when conventional stirred-tank impellers are employed. To address this limitation, alternative reactor configurations, such as Oscillatory Baffled Reactors (OBRs), have been proposed. OBRs employ strategically positioned baffles combined with oscillatory flow to enhance mixing performance under laminar flow conditions, making them particularly well suited for processing highly viscous slurries [95].

A further challenge arises from the differing optimal operating temperatures of the biocatalysts involved in the SSF process. Cellulolytic enzymes typically exhibit maximum

activity at approximately 50 °C, whereas fermentative microorganisms perform optimally at around 35 °C. Consequently, SSF requires operation at an intermediate temperature, representing a compromise that inevitably reduces the efficiency of one or both biological processes and may lead to lower ethanol yields. Although separating enzymatic hydrolysis and fermentation into sequential processing steps would allow each stage to operate under its respective optimum conditions, thereby enhancing reaction kinetics and overall conversion, this strategy sacrifices the inherent advantages of SSF. These include reduced end-product inhibition, lower capital and operating costs through process integration, decreased contamination risk, and simplified process operation. Accordingly, careful optimisation of reactor design and operating conditions is essential to balance these competing considerations and achieve efficient, economically viable large-scale bioethanol production.

7. Recommendations

7.1. Process Optimisation Opportunities

This styrene process can be further optimised, as it is currently constrained by limitations present during the design of the current styrene plant. One such optimisation is the implementation of a reactive distillation column when synthesising ethylbenzene instead of a plug flow reactor, followed by a distillation column setup. Not only does this optimisation save on capital costs, as there will be a reduction in the amount of equipment required, but it also increases the conversion of the reactants to ethylbenzene due to the shift in equilibrium to the product side, as well as improved selectivity, which could nullify the need to separate and react diethylbenzene to form a higher quantity of ethylbenzene [96]. In the end, we opted for the separate PFR and distillation column due to the complexity of the design and the time constraint on the design team.

Additionally, the bacterial strains, *S. cerevisiae* D5A and *E. coli* KO11, can be substituted for a single bacterial strain that is genetically modified to allow the fermentation of both hexose and pentose sugars. The *rZymomonas mobilis* 13-H-9-2 bacteria synthesised by NREL is ideal for this process due to its high conversion rate, resulting in high ethanol titres of around 70 g/L [26,97]. *rZymomonas mobilis* 13-H-9-2 was originally considered for this process during the conceptual design phase but was substituted by *S. cerevisiae* D5A and *E. coli* KO11 because *rZymomonas mobilis* 13-H-9-2 was not industrially available at the time, and additional projects that use the strain had a member from the NREL team as part of the project. By using this strain, there could be a slight rise in cost, depending on the cost of the strain when it becomes available, but this would count towards our capital costs, as bacteria will be a one-time purchase, and we can continuously grow the bacteria in the laboratory. However, capital costs can also decrease due to only requiring one fermentation tank to grow the bacterial strain instead of two, as well as a reduction in operational costs as fewer nutrients would be required as there is now only one bacterial strain to ‘feed.’ Overall, it is an optimisation that is unlikely to significantly change the calculated economics of the process while reaping the benefits of its high ethanol titres.

7.2. Tech Scale-Up Considerations

While the proposed design effectively demonstrates the technical and sustainability principles at a conceptual or pilot scale, scaling up to industrial production introduces a new set of challenges and considerations. Key factors include the availability and logistics of biomass feedstock (corn stover) at large volumes, consistent catalyst performance over extended operating cycles, and integration of heat recovery systems across expanded process units. Equipment sizing must account for increased flow rates, pressure drops, and energy demands, requiring rigorous scale-up correlations and pilot testing data. Additionally, continuous reactor operation, especially for catalytic alkylation and dehydrogenation,

must be evaluated for residence time distribution, fouling tendencies, and thermal management at scale. Regulatory compliance, particularly concerning emissions and effluent management, becomes more stringent at higher production capacities. Finally, scale-up must consider supply chain integration for ethanol production, benzene procurement, and styrene storage, with sensitivity analysis for market fluctuations.

Transitioning from a conceptual design to full-scale industrial implementation involves a range of technical and logistical challenges. For the sustainable styrene process presented, the scale-up must address process robustness, supply chain integration, and capital-intensive infrastructure development. This section outlines the key barriers and enablers to effective scale-up, with particular focus on catalyst longevity, equipment scalability, and the policy landscape.

A major challenge in scaling up the alkylation and dehydrogenation stages is the potential for catalyst deactivation due to fouling, coke formation, or poisoning by impurities in the biomass-derived ethanol. While beta-zeolite and iron oxide catalysts demonstrate strong selectivity at the lab scale, their performance under continuous industrial operation over prolonged periods requires thorough evaluation. Catalyst regeneration protocols, material resilience, and periodic replacement cycles must be optimised to maintain efficiency and minimise downtime. Pilot-scale studies and reactor modelling can help predict catalyst life and inform inventory and cost planning at the commercial scale.

At an industrial scale, the design of reactors, heat exchangers, and separation units must consider not only increased throughput but also mechanical and thermal stress tolerance. Fabricating reactors capable of handling high temperatures and pressures, especially for the endothermic dehydrogenation of ethylbenzene, demands precise material selection and engineering standards. Additionally, scale-up affects control systems, instrumentation layout, and safety mechanisms, all of which must be reconfigured for larger operating envelopes. Modular design strategies and prefabricated skids may offer advantages in reducing construction time and improving quality control.

Wider deployment of bio-based chemical production technologies is heavily influenced by supportive government policies. For this project, scale-up success is likely to depend on access to renewable energy subsidies, green technology grants, and preferential tax schemes. In regions where bioethanol production is already incentivised (e.g., India's Ethanol Blended Petrol programme), co-locating styrene facilities near ethanol hubs could reduce feedstock costs and transport emissions. Additionally, aligning with national sustainability goals or SDG-aligned development plans could open avenues for public-private partnerships, accelerating the transition from pilot to full-scale deployment.

7.3. Policy and Incentive Opportunities

The success of such large-scale sustainable chemical manufacturing is linked to the availability of supportive policy frameworks and government incentives. In the context of bio-based styrene production, policy mechanisms such as renewable energy subsidies, tax credits for green technology investment, and carbon pricing schemes can significantly improve the economic viability of scale-up. Many countries offer feed-in tariffs or capital grants for facilities that integrate renewable energy sources, which could offset the high thermal energy demand in the styrene dehydrogenation step. Tax credits for renewable feedstocks or clean-tech infrastructure, such as India's Production Linked Incentive (PLI) scheme for biofuels or the U.S. Section 45Q tax credit for carbon capture, may apply to key components of the plant. Carbon trading or offset programmes could also provide financial value for reduced GHG emissions achieved by diverting biomass waste from open burning. Furthermore, policies that promote industrial symbiosis and biorefinery clusters could facilitate shared logistics and infrastructure, which would reduce costs for both ethanol

sourcing and waste valorisation. Strategic alignment with national sustainability agendas and SDG targets could strengthen the case for public funding or regulatory prioritisation of such innovative projects.

Some national incentives available in India include:

Production Linked Incentive (PLI) Scheme for Biobased Chemicals

Under India's PLI framework, projects producing eligible biobased chemicals like biostyrene intermediates can receive direct financial incentives tied to incremental sales, making commercialisation more attractive.

Accelerated Depreciation and Generation-Based Incentives (GBI)

Renewable energy investments are supported through accelerated depreciation, generation-based incentives (~₹0.50/kWh for wind/solar), and customs/excise duty waivers on clean-energy equipment. These reduce capital costs for solar/wind installations that can power the styrene process.

Section 115BAB Concessional Tax Rate

New manufacturing units may qualify for a lower corporate tax rate of 15% (effective ~17.2%) under Section 115BAB if conditions are met, though updates post-March 2024 should be confirmed.

Gujarat-State and Surat-Specific Advantages

- **Industrial Policy 2020 (MSME and Large Industry Incentives)**
Gujarat offers interest subvention on term loans (5–7%, up to ₹35 lakh/yr), SGST reimbursement (up to 100% for 10–20 years), EPF rebates, and capital subsidies ranging from 10 to 25% of investment. These incentives significantly reduce financing and operational costs.
- **Green/Sustainability Equipment Support**
State nodal bodies may offer additional support for clean-technology systems, including exemptions or grants for installing energy-efficient reactors and waste-treatment setups.
- **Renewable Energy and Captive Power Support**
Under Gujarat's Renewable Energy Policy 2023-28, large industrial users in Surat can harness open-access solar/wind energy with banking through distribution companies and duty exemptions ideal for powering high-energy steps like dehydrogenation.
- **Special MSME Start-up Perks**
Registered startups and MSMEs can enjoy extra interest relief (1%), seed and sustenance funding, electricity duty waivers (5 years), stamp duty reimbursement, and marketing grants delivered through the Udyam registration and IFP portal.

8. Key Design Outcomes

- A sustainability-focused styrene production plant was designed by integrating conventional ethylbenzene dehydrogenation with bioethanol derived from agricultural corn stover, demonstrating a viable low-carbon alternative to fossil-based feedstocks.
- Bioethanol production using two-phase simultaneous saccharification and fermentation achieved yields of up to 477 kg per tonne of corn stover, enabling high-efficiency downstream conversion to ethylbenzene and styrene.
- High process performance was achieved, with ethylbenzene conversion of 95%, styrene selectivity of 96.2%, extensive benzene recycling, and integrated heat recovery, supporting an annual production capacity of 220,000 tonnes per year.
- Strategic location in Gujarat leverages local biomass availability, skilled labour, infrastructure, and cost advantages, while supporting regional development and alignment with UN Sustainable Development Goals.

- Comprehensive safety measures, including advanced fire prevention, continuous gas monitoring, and secure chemical handling, mitigate hazards associated with flammable and toxic materials.
- Techno-economic analysis confirms strong commercial viability, with a capital investment of \$265 M USD, an estimated payback period of under three years, and projected post-tax annual profits of \$45.7 M USD.
- As a case study, the work provides a concise and transferable framework for teaching sustainability-led process design, integrating technical rigour, safety, waste valorisation and economic decision-making within chemical engineering curricula.
- Overall, the design delivers a sustainable, economically viable, and socially beneficial pathway for styrene manufacture—setting a benchmark for how chemical engineering innovation can drive progress toward a low-carbon and circular economy.

9. Conclusions

This study demonstrates the technical feasibility and economic viability of a sustainability-driven styrene production process that integrates renewable bioethanol within a conventional petrochemical framework. The proposed approach provides a credible pathway for low-carbon, resource-efficient styrene production without compromising industrial performance, with an estimated ten-fold reduction in CO₂ emissions compared to the conventional styrene production process. The results confirm that renewable carbon can be effectively incorporated into large-scale chemical manufacturing. High conversion and selectivity across key process stages, combined with systematic material and energy integration, including reactive distillation, benzene recycling, and heat recovery, significantly enhance process efficiency while reducing emissions and utility demand.

The strategic selection of Gujarat, India, highlights the importance of contextual design, leveraging regional biomass availability and infrastructure to strengthen supply chain resilience and support local economic development. Importantly, the short payback period and strong post-tax profitability directly challenge the prevailing assumption that sustainable technologies entail economic sacrifice. Instead, the findings show that process intensification, integration, and careful design optimisation can deliver both environmental and financial gains, as demonstrated with an ROI of 17.2%, IRR of 28% and NPV of \$1830 M. This case study, therefore, provides a compelling model for future industrial implementation, illustrating how sustainability, safety, and profitability can be simultaneously realised in next-generation chemical process design, addressing the UN's sustainable development goals, in particular SDG 7 (affordable and clean energy), SDG 12 (responsible consumption and production) and SDG 13 (climate action).

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