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Energy and Economic Viability of Hybrid Biorefineries: A Comparative Study between Hydrogen−Sustainable Aviation Fuel and Hydrogen−Ethanol Pathways

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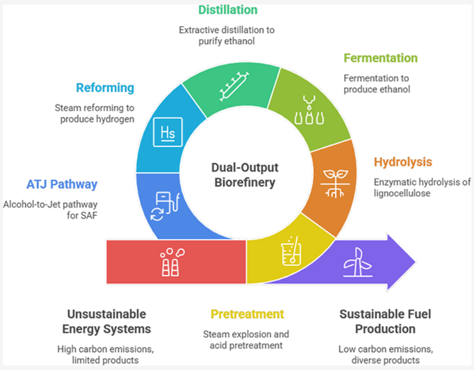
ABSTRACT: In the pursuit of a sustainable and circular bioeconomy, the integration of hydrogen production into lignocellulosic biorefineries offers a promising strategy for decarbonizing energy systems and diversifying value-added products. This study proposes and evaluates a flexible, dual-output biorefinery capable of producing either sustainable aviation fuel (SAF) and hydrogen or ethanol and hydrogen, using bagasse and corn stover as feedstocks. A comprehensive process simulation was conducted in Aspen Plus, including steam explosion and acid pretreatment, enzymatic hydrolysis, fermentation, extractive distillation, steam reforming, and the Alcohol-to-Jet (ATJ) pathway. Techno-economic and environmental performance were assessed using Return on Investment (ROI) and CO_2 emissions as key metrics. Results show that the ethanol−hydrogen configuration presents at least one economically viable scenario under current market conditions without requiring electrification of heat-demanding operations. Conversely, the SAF−hydrogen route is not economically feasible under base conditions, although its performance improves significantly when the thermal energy demand is eliminated through electrification. Sensitivity analyses of product selling prices demonstrate that modest increases in the SAF, hydrogen, or ethanol prices could make the proposed system viable. The study highlights the potential of adaptive biorefinery architectures to respond to shifting geopolitical and market conditions, supporting resilient and sustainable fuel production strategies.



1. INTRODUCTION

The aviation industry, a vital component of the global economy and connectivity, faces a profound challenge: the urgent need to decarbonize its operations. Historically reliant on fossil fuels, aviation has emerged as a significant contributor to global CO_2 emissions, necessitating a fundamental transformation in its energy sources.[1] As environmental awareness intensifies and climate regulations become more stringent, the pressure on the sector to reduce greenhouse gas (GHG) emissions is escalating. The projected growth in air traffic further exacerbates this situation, making the pursuit of clean and renewable energy alternatives for the aviation sector an imperative.

Sustainable Aviation Fuel (SAF) offers up to 70% lifecycle GHG reduction relative to conventional jet fuel and is fully compatible with current aircraft and fuel infrastructure.[2] These characteristics make SAF an essential reference point for evaluating the environmental performance of the configurations analyzed in this study.

Several technological pathways have achieved regulatory approval under ASTM D7566, most notably: Hydroprocessed Esters and Fatty Acids (HEFA), Fischer−Tropsch (FT) synthesis (also known as FT-SPK), and Alcohol-to-Jet (ATJ) routes (Figure 1). Each approach offers distinct advantages and challenges:

- HEFA is currently the most mature and widely deployed technology, leveraging fats and oils to produce paraffinic hydrocarbons with robust energy characteristics as lower sulfur and aromatic content, higher cetane rating than conventional aviation fuel, and the possibility to be blended up to 50% with conventional aviation fuel.[3] However, feedstock constraints and competition with food and oleochemical industries limit scalability and raise sustainability concerns.
- FT-SPK enables high GHG abatement (often below 12 gCO_2e/MJ) and utilizes versatile biomass feeds, including municipal solid waste.[4] Despite these merits, FT-SPK demands high capital investments, complex

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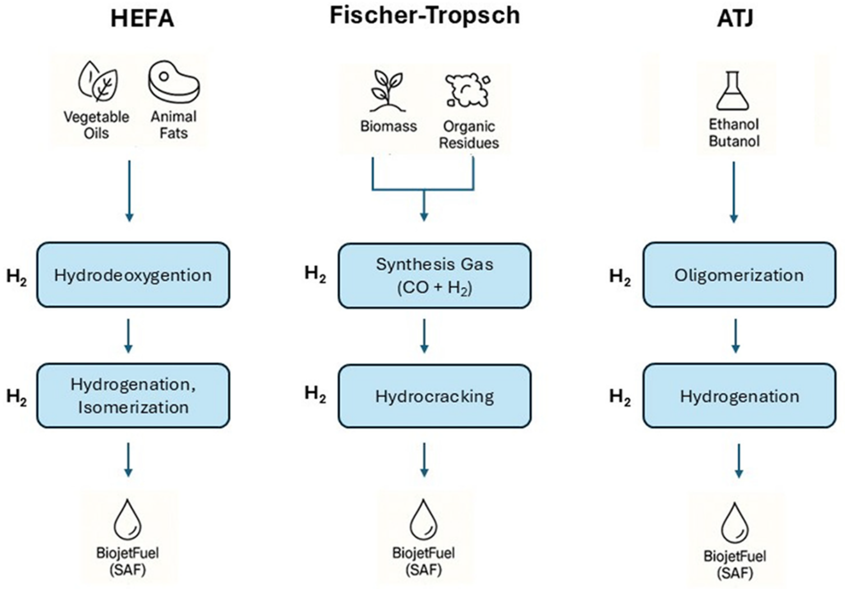

Figure 1. Alternative Routes to produce SAF.

syngas production systems, and extensive downstream cleanup and upgrading units.

ATJ, in contrast, converts short-chain alcohols (e.g., ethanol, isobutanol) into jet-range hydrocarbons (C_8 to C_{16}) and offers superior feedstock flexibility (ranging from sugar and starch to lignocellulosic residues) and modular processing units. Alcohols can be obtained utilizing biochemical processes such as fermentation and thermochemical processes such as pyrolysis and gasification.[5] Recent lifecycle analyses and techno-economic studies indicate that ATJ-SPK can deliver high carbon reductions with favorable returns: lifecycle GHG footprints often fall below 24 g of CO_2 eq/MJ or feedstocks such as sugar cane and forestry residues,[6] and return on investment can reach 13.7%[7] owing to lower-cost precursors like bioethanol. Besides the notable reduction of CO_2 emissions, ATJ has a higher production cost than HEFA, depending on the raw material, but lower than FT-SPK.[8] However, the wide range of raw materials that can be used by the ATJ route without compromising land use and feeding the population gives it an advantage. Moreover, ATJ's modular design facilitates smaller-scale, decentralized facilities—ideal for regions with distributed biomass resources—thus mitigating logistics and infrastructure costs.[9]

For these reasons, namely, feedstock diversity, modular implementation, strong environmental performance, and economic viability, ATJ is increasingly regarded as one of the most promising routes for large-scale SAF deployment.[10] Within the SAF landscape, hydrogen, often a hidden or implicit player, warrants focused analysis due to its fundamental and multifaceted role. Hydrogen plays a multifunctional and essential role in SAF production across all of the major technological pathways. Beyond its future potential as an aviation fuel, hydrogen is required both as an energy vector, supplying heat and power for key conversion steps, and as a chemical reactant that drives critical upgrading reactions. In processes such as hydrogenation and hydrodeoxygenation,[11] hydrogen improves fuel stability, removes oxygenated groups, and enables the formation of high-quality paraffinic hydrocarbons. Although its specific use varies by route, extensive hydrodeoxygenation in HEFA, syngas conversion in Fischer–Tropsch synthesis,[12] and final-stage hydrogenation in the ATJ pathway,[13] each technology relies on hydrogen availability, purity, and pressure to meet jet fuel specifications and ensure overall process sustainability.

The origin of hydrogen is as important as its function. The use of green hydrogen, produced through water electrolysis using renewable energy (solar and wind), is fundamental to maximizing the sustainability of SAF. The integration of green hydrogen into biojet fuel production not only reduces emissions associated with hydrogen production itself but also fosters a circular economy by closing the carbon loop and minimizing reliance on fossil fuels. This synergy between green hydrogen and SAF production represents a significant step toward truly sustainable aviation and a more circular economy. The large-scale implementation of SAF and green hydrogen is being driven by policy frameworks and regulations at the global level. Initiatives such as the International Civil Aviation Organization's (ICAO) Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA), the European Union's ReFuelEU Aviation initiative, and the Inflation Reduction Act (IRA) in the United States establish targets and support mechanisms for SAF production and use. These policies not only create a favorable environment for investment in SAF and hydrogen technologies but also incentivize the research and development of innovative solutions for aviation decarbonization. Alignment with these regulatory frameworks is crucial for the success and expansion of hydrogen-enabled biojet fuel production.

The simultaneous evaluation of the hydrogen–SAF and hydrogen–ethanol configurations does not intend to compare them as competing or mutually exclusive options. Instead, both pathways are conceived as complementary routes within a single, flexible biorefinery framework. They share common feedstock supply, pretreatment operations, utilities, and hydrogen production units while differing only in their downstream conversion and product valorization strategies. Assessing both scenarios under a unified simulation and evaluation methodology enables the identification of cross-process synergies, shared infrastructure benefits, and operational trade-offs. This integrative perspective reflects the real-world design logic of emerging multioutput biorefineries, where modular production routes can adapt to market fluctuations, policy incentives, or sustainability targets. Therefore, the purpose of merging the two configurations in this study is to provide a holistic, system-level comparison that clarifies the relative advantages of each hydrogen utilization strategy within the broader context of SAF and bioethanol production.

With all of this background in mind, this review aims to elucidate the central role of hydrogen as both an energy vector and a chemical reactant in the ATJ route for SAF production. It will delve into each stage of the ATJ process where hydrogen is fundamental, highlighting its influence on fuel quality, process efficiency, and sustainability profile. Furthermore, critical requirements will be discussed as well as their impact on the technical and economic feasibility of large-scale ATJ deployment. This analysis seeks to provide a comprehensive understanding of the indispensable role of hydrogen in the transition toward more sustainable aviation. Building upon this framework, the main objectives of this study are threefold: (i) to design and simulate an integrated lignocellulosic biorefinery capable of coproducing hydrogen with either SAF or ethanol; (ii) to conduct a rigorous techno-economic and environmental evaluation of both configurations under representative Mexican conditions; and (iii) to identify the operating and market conditions that render each configuration economically and environmentally feasible. These objectives provide a structured pathway to assess how hydrogen valorization can strengthen the viability and sustainability of SAF production systems.

The novelty and scientific contribution of this work lie in its comparative, system-level techno-economic assessment of two dual-output biorefineries using a unified simulation framework. Unlike previous studies that have analyzed these configurations independently, this research integrates process design, energy analysis, and environmental and economic modeling into a single consistent methodological approach. This unified assessment allows quantification of trade-offs among hydrogen allocation, process electrification, and product market value, offering new insights into the optimal strategies for hydrogen utilization in SAF-related biorefinery systems. Moreover, the methodological integration proposed here establishes a foundation for future research involving multiobjective optimization and uncertainty analysis to further enhance process robustness and decision reliability.

2. HYDROGEN UTILIZATION AND INTEGRATION STRATEGIES IN THE ATJ PATHWAY

The ATJ pathway represents one of the most technologically mature approaches for SAF production, with a Technology Readiness Level (TRL) of 8−9.[14] This pathway converts biomass-derived alcohols (typically ethanol or isobutanol) into fully formulated synthetic paraffinic kerosene (SPK) that meets strict ASTM D7566 specifications for aviation fuel.[15] The ATJ process involves four major steps: (1) alcohol production via fermentation of sugars (from sugar cane, corn, or lignocellulosic biomass), (2) alcohol dehydration to olefins, (3) oligomerization of light olefins to heavier hydrocarbons, and (4) hydrogenation of oligomers to produce saturated isoparaffins suitable as jet fuel.[13]

In the alcohol-to-jet (ATJ) conversion pathway, hydrogen plays a vital role in the final processing step: the catalytic hydrogenation of oligomerized alcohol intermediates. In this stage, hydrogen is introduced over a suitable catalyst to saturate the olefinic double bonds formed during oligomerization, thereby converting unsaturated hydrocarbon chains into fully saturated paraffinic hydrocarbons that meet jet fuel specifications.[1] This hydrogenation step is essential for fuel stability and performance, yielding a low-reactivity, high-quality jet fuel product with the required combustion characteristics and storage properties.[13] The hydrogen consumption varies significantly based on feedstock and process design, typically ranging from 0.02 to 0.05 kg per liter of biojet fuel produced.[14] This work synthesizes current scientific understanding of hydrogen's multidimensional impacts across energy systems, economic viability, and environmental performance in ATJ biojet fuel production.

However, the source of hydrogen used in this step significantly affects the overall energy efficiency of the ATJ process. Industrial hydrogen is predominantly produced via steam methane reforming (SMR) of natural gas, an energy-intensive, fossil-based method, and the provision of this hydrogen can be one of the largest contributors to the life-cycle emissions and fossil energy input of biojet fuel production. Life-cycle assessments have shown that ATJ fuels utilizing conventional SMR-derived hydrogen achieve substantially smaller greenhouse gas reductions compared with those using renewable hydrogen sources. For instance, in a comparative analysis of biojet pathways, an ATJ-related process was found to reduce GHG emissions by only ∼ 28% relative to petroleum jet fuel when using hydrogen from natural gas SMR, versus a ∼ 71% reduction when using hydrogen produced via biomass gasification.[2] This stark contrast underscores how the hydrogen source is a critical lever for improving the energy efficiency and net renewable fraction of ATJ-derived biojet fuels, making the integration of low-carbon hydrogen (e.g., from renewable electrolysis or biomass-based processes) imperative for truly sustainable aviation fuel production.

Current industrial hydrogen production predominantly relies on steam methane reforming (SMR), which utilizes natural gas and has an energy intensity of approximately 200−250 MJ per kg of H_2 produced.[16] When SMR-derived hydrogen is used in ATJ processes, it substantially reduces the lifetime renewability of the biojet fuel. Alternative pathways include:

- Biomass Gasification: Production of biosyngas followed by water−gas shift to generate renewable hydrogen
- Electrolysis: Using renewable electricity to split water, providing zero-emission hydrogen
- Byproduct Hydrogen: Utilization of hydrogen from industrial processes (e.g., chlor-alkali plants)

A comparative analysis shows that ATJ systems utilizing grid electrolysis hydrogen exhibit 15−20% lower overall energy efficiency compared to SMR-based systems due to electricity conversion losses.[16] However, when renewable-powered electrolysis is employed, the fossil energy input decreases dramatically, improving the renewable energy ratio of the final fuel.

Recent innovations focus on thermal integration and hydrogen recovery to minimize energy penalties. Villareal-Hernández et al.[13] demonstrated that intensifying the oligomerization and hydrogenation stages through optimized heat integration could reduce energy consumption by 12−18% in the ATJ process. Additionally, implementing membrane separation technologies for hydrogen recovery from purge gases can improve the hydrogen utilization efficiency by 20–25%. Table 1 summarizes energy metrics for different hydrogen integration approaches. ATJ system efficiency, expressed in percentage, is defined as the ratio between the energy content of the final biojet fuel and the total energy supplied to the ATJ pathway. This is the total energy includes the chemical energy of the alcohol feedstock, the supplemental hydrogen required during oligomerization, hydrotreatment, and all thermal and electrical input to the process. Higher values indicate a more efficient conversion of energy inputs into usable jet fuel. On the other hand, the fossil energy ratio (FER) is a dimensionless indicator that measures the share of renewable energy in the produced fuel relative to the fossil energy consumed along its production chain. It is calculated as the ratio of the renewable energy contained in the final biojet fuel to the cumulative fossil energy required for the feedstock production, hydrogen generation, and process operation, so lower values reflect a higher like 0.5–0.7 correspond to dependence on fossil energy, while values approaching indicate reduced fossil energy dependence.

Table 1. Hydrogen Integration Approaches[16]

Hydrogen Source	Energy Intensity (MJ/kg H_2)	ATJ System Efficiency	Fossil Energy Ratio
SMR (Natural Gas)	200–250	58–62%	0.65–0.75
Grid Electrolysis	110–140 (elec. equivalent)	45–52%	0.50–0.60
Solar Electrolysis	90–110 (elec. equivalent)	54–58%	0.85–0.92
Biomass Gasification	160–190	60–65%	0.92–0.98

Techno-economic analyses consistently identify hydrogen supply as a major cost driver in ATJ biojet fuel production, typically representing 15–25% of the operating expenses. For a standard ATJ plant processing 360 kg/h of biojet fuel (approximately 6.8 barrels/day), the annual hydrogen cost ranges between \$1.2–\$2.0 million, assuming current market prices of \$2.5–\$4.0/kg for renewable hydrogen. The total capital investment for such facilities is estimated at \$60-\$80 million, with the hydrogenation unit contributing 12–18% of equipment costs.[14] Economic viability is highly sensitive to hydrogen pricing. Studies in the Mexican context indicate that reducing hydrogen costs below \$2.0/kg could improve the Return on Investment (ROI) for ATJ facilities from the current baseline of 13.7% to over 16%, making it competitive with petroleum-derived jet fuels at oil prices above \$80/barrel.[14] This underscores the critical need for cost reductions in clean hydrogen production to enhance ATJ commercial viability.

The economies of scale significantly impact ATJ economics, with larger facilities (1,000+ barrels/day) potentially reducing hydrogen-related costs through bulk procurement and on-site production. Process intensification strategies proposed by Villareal-Hernández et al.[13] demonstrate potential for 20–30% capital cost reduction in hydrogenation units through reactor optimization and advanced catalysts. These improvements could decrease the minimum selling price of ATJ biojet fuel from the current \$1,200–\$1,500/ton to \$900–\$1,100/ton, approaching cost-competitiveness with conventional jet fuel.[14]

On the other hand, Life Cycle Assessment (LCA) studies reveal that hydrogen sources critically determine the environmental benefits of ATJ biofuels. When produced via SMR, hydrogen contributes 40–50% of the total cradle-to-grave emissions of the ATJ biojet fuel. This results in a Global Warming Potential (GWP) of approximately 60–70 g CO_2-eq/MJ—significantly better than conventional jet fuel (89 g CO_2-eq/MJ) but substantially higher than pathways like HEFA at 43.6 g CO_2-eq/MJ.[16] Switching to renewable hydrogen dramatically improves this performance:

- Solar Electrolysis Hydrogen: Reduces GWP to 25–35 g CO_2-eq/MJ
- Biomass-Derived Hydrogen: Achieves GWP as low as 15–25 g CO_2-eq/MJ
- Grid Electrolysis (Renewable-heavy mix): 30–40 g CO_2-eq/MJ

These emissions represent 60–80% reductions compared to conventional jet fuel when renewable hydrogen is utilized.[17] Importantly, ATJ pathways using cellulosic biomass and renewable hydrogen achieve near-zero or even negative emissions when carbon sequestration during biomass growth is accounted for.[16]

Beyond climate impacts, hydrogen choices influence multiple environmental dimensions:

- Water Consumption: Electrolysis-based hydrogen increases water use by 3–5 L/kg fuel compared to SMR hydrogen.[16]
- Land Use Change: Utilizing waste-derived hydrogen avoids the indirect land use change (iLUC) emissions associated with biomass cultivation.
- Air Quality: ATJ fuels with complete hydrogenation reduce particulate matter (PM) emissions by 50–70% and sulfur oxides (SO_x) by nearly 100% compared to conventional jet fuel.
- Contrail Formation: Fully hydrogenated ATJ fuels demonstrate reduced soot emissions, potentially decreasing contrail formation and associated radiative forcing.[17]

Hydrogen thus plays an essential role in the successful production of SAF, particularly within the ATJ pathway. It is not only essential for achieving the required fuel properties but also serves as a determinant of the overall energy efficiency, environmental performance, and economic viability of the ATJ process. However, a critical observation drawn from the current body of literature is that most studies focus exclusively on hydrogen as an external input or isolated process variable. These analyses often overlook the broader system-level integration opportunities that arise within biorefinery configurations. Although some alternatives for in situ hydrogen production have been reported, such as aqueous phase reforming under milder conditions (220–270 °C and 30–60 bar), which have the advantage of avoiding the need to vaporize water, thereby reducing energy requirements.[18,19]

Other techno-economic analyses of the Alcohol-to-Jet (ATJ) pathway have been extensively reported using various feedstocks, along with life cycle assessments (LCAs) to evaluate the environmental impacts of the process.[20−24] These studies reveal significant variations in both economic and environmental outcomes across the different cases. Yang et al.[25] conducted a comprehensive uncertainty analysis for multiple SAF pathways, including ATJ, identifying the hydrogen source as the main driver of variability in both cost and environmental performance. They also highlighted the cost of alcohol

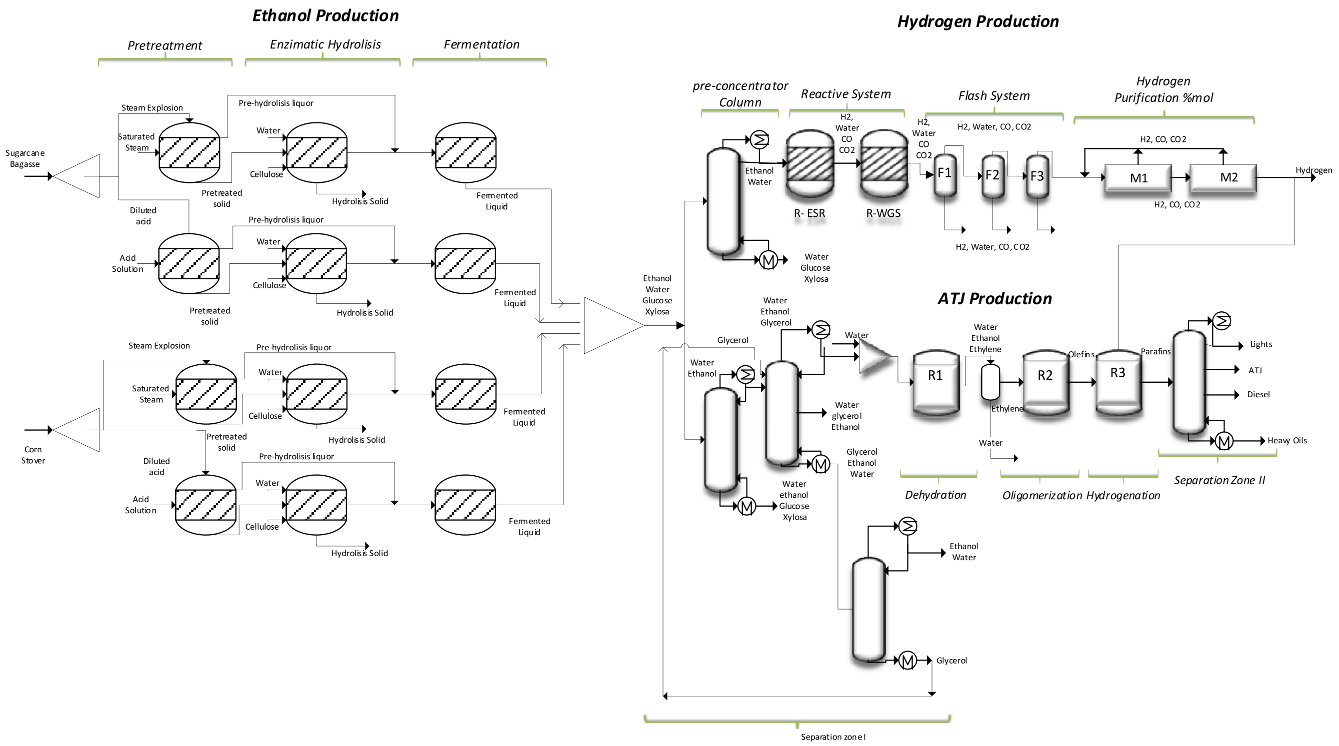

Figure 2. Flowsheet of the ATJ process from biomass

feedstock as the major limitation for improving ATJ process economics, a conclusion consistent with other studies.[26,27] Hong et al.[28] proposed a lignocellulosic-based route for jet fuel production through biomass conversion and C−C coupling of aqueous ethanol, utilizing wheat straw and industrial cellulose residues. Similarly, Uddin et al.[29] simultaneously evaluated the economic and environmental performance of the ethanol-to-jet fuel pathway using corn stover and corn grain as feedstocks. Kourkoumpas et al.[30] presented a case study of retrofitting a bioethanol plant to produce SAF through the ATJ route, demonstrating the potential for technological integration within existing infrastructures. On a broader scale, Bedin et al.[31] analyzed the impact of SAF production through the ATJ route from lignocellulosic biomass in the European context, addressing issues of scalability and national potential to meet aviation fuel demand. Bianco et al.[32] investigated how regional geography influences the profitability of the ethanol-to-SAF process in the United States, considering the end-to-end supply chain and providing insights into potential trade-offs between cost and sustainability.

In particular, integrated biorefineries based on lignocellulosic biomass, such as the ATJ process from ethanol, offer unique potential: the concurrent production of ethanol, hydrogen, and SAF within a single facility. This coproduction approach opens the door to more circular and energy-efficient schemes, where hydrogen can be generated on-site (e.g., via ethanol reforming or biomass gasification) and immediately utilized within the hydrogenation step of the ATJ process. Despite its promise, this integrated strategy raises new questions regarding process optimization, hydrogen allocation, and economic trade-offs.

Which configuration provides the most technically feasible, economically competitive, and environmentally sustainable route for SAF production? This proposal seeks to address that question by evaluating various coproduction scenarios, assessing their performance across technical, economic, and environmental dimensions. Through this systems-level analysis, a more comprehensive understanding of hydrogen's strategic role in integrated ATJ biorefineries will be developed.

3. CASE STUDY: INTEGRATED BIOREFINERY FOR THE COPRODUCTION OF ETHANOL, HYDROGEN, AND SAF

In this work, a regional case study in Mexico is proposed. Mexico presents a highly suitable context for implementing an integrated biorefinery that coproduces bioethanol, hydrogen, and SAF. This suitability is underpinned by three key factors: abundant biomass availability, supportive energy infrastructure, and a conducive regulatory framework. Mexico generates approximately 800 million tons of biomass annually, encompassing agricultural residues, forest byproducts, and organic waste. This substantial biomass potential positions the country as a significant player in biomass-based energy production, including biogas and biofuels.[33]

Mexico's commitment to clean energy is reflected in its policies and reforms. The National Development Plan (2025−2030) emphasizes energy sovereignty and the integration of clean and renewable energy across all stages of the value chain. Furthermore, the enactment of new energy laws in 2025 aims to strengthen the role of state-owned enterprises in the energy sector, promoting a stable and supportive environment for renewable energy projects. These factors collectively create a favorable environment for the proposed integrated biorefinery in Mexico, aligning with the country's strategic objectives in energy sustainability and economic development.[34]

Figure 2 illustrates the main process flow of the integrated biomass-to-jet fuel system. The figure shows the sequential stages, including pretreatment, hydrolysis, fermentation, hydrogen production, and the alcohol-to-Jet (ATJ) upgrading step. The integrated concept allows the conversion of lignocellulosic biomass into bioethanol, hydrogen, and ultimately jet fuel

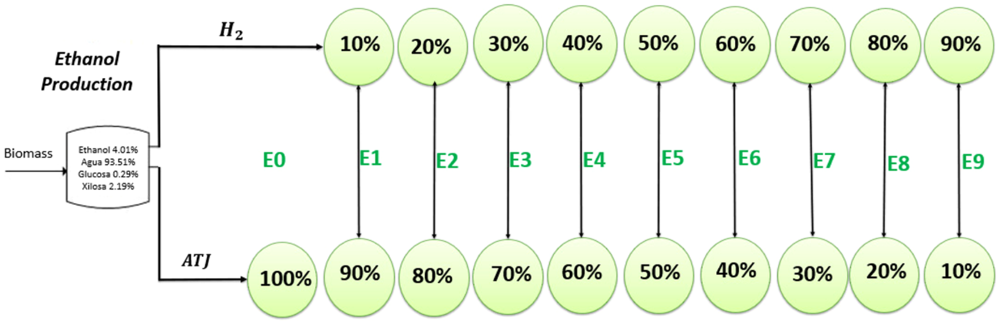

Figure 3. Proposed scenarios for the simultaneous production of hydrogen and SAF from biomass; all scenarios consider wt % intervals.

through catalytic hydrogenation. This integrated design aims to maximize hydrogen utilization and process efficiency. The following sections discuss each of these steps in detail. As illustrated in Figure 2, the integrated biomass-to-jet fuel system combines all main conversion steps, enabling efficient hydrogen valorization and process intensification.

The process design was adapted to the biomass availability in central Mexico, considering an annual feedstock supply of 1,330,000 tons of corn stover and 7,488,376 tons of sugar cane bagasse from the states of Guanajuato, Michoacán, San Luis Potosí, Jalisco, Querétaro, and Zacatecas. The integration of renewable feedstocks and advanced catalytic and separation technologies positions this ATJ-based system as a promising approach to decarbonizing the aviation sector. The integrated process shown in Figure 2 is briefly described below.

3.1. Process Description

3.1.1. Ethanol Production from Biomass. The ethanol production process initiates with the pretreatment of lignocellulosic biomass through steam explosion. This process was assumed to occur at 190 °C and 1 MPa to promote partial depolymerization of hemicellulose and disruption of lignin–carbohydrate complexes. Under these conditions, xylan solubilization reaches 85%, while cellulose digestibility increases from <20% (raw biomass) to 75% after pretreatment.[35,36] Subsequent dilute-acid washing with 0.5 wt % H_2SO_4 at 130 °C improves hemicellulose hydrolysis, achieving xylose yields of 80%.[37]

The pretreated biomass undergoes enzymatic hydrolysis using cellulase and hemicellulase to release fermentable sugars, primarily glucose and xylose. These sugars are subsequently fermented by *Saccharomyces cerevisiae* or engineered Zymomonas mobiliz to produce ethanol.[38] Enzymatic hydrolysis was modeled considering 50 °C, pH.[45] Literature indicates that under these conditions, glucose yields of 90% and xylose yields of 80% can be obtained for pretreated agricultural residues.[39]

After fermentation, the ethanol-rich broth is purified via a two-stage distillation sequence. A prefractionation column first concentrates ethanol to approximately 94 wt %, separating it from water and residual byproducts. The concentrated stream is then fed into an extractive distillation column using glycerol as an entrainer, which increased the relative volatility between ethanol and water. This configuration enables ethanol purification up to 99.5 wt %, fulfilling the quality requirements for both hydrogen production and subsequent processing in the ATJ pathway.[40]

3.1.2. Hydrogen Production via Ethanol Steam Reforming. Hydrogen is generated from ethanol through a two-step thermochemical route comprising steam reforming and Water–Gas Shift (WGS) reactions. In the first step, concentrated ethanol reacts with steam over a $Ni/MgO/Al_2O_3$ catalyst at 600–800 °C, producing a synthesis gas mixture of hydrogen, carbon monoxide, carbon dioxide, and unreacted steam.[41] The syngas is then processed in a WGS reactor at around 400 °C using a $CuO/ZnO/Al_2O_3$ catalyst to convert residual CO and steam into additional hydrogen and CO_2, enhancing the overall hydrogen yield. The resulting gas stream is purified by sequential flash separators and two membrane units made of Matrimid polymer. These membranes selectively permeate hydrogen, achieving a final purity of ≥ 99 mol %, suitable for use in the ATJ hydrogenation step.[42]

3.1.3. ATJ Production. The ATJ route begins with the catalytic dehydration of ethanol to ethylene over solid acid catalysts such as γ-Al_2O_3 or zeolites at 300–450 °C and moderate pressure (1–3 bar). Ethanol dehydration achieves complete or near-complete ethanol conversion with ethylene selectivities above 90–100% under optimized conditions (220–300 °C), providing a clean C_2 feed for downstream oligomerization.[43] Ethylene is then oligomerized into C_8–C_{12} hydrocarbons over solid acid catalysts like H-ZSM-5 or SAPO-11 in a fixed-bed reactor, operated at 150–300 °C and 20–60 bar.[44] Ethylene oligomerization on bifunctional acid catalysts has been reported to reach 98–99 mol % ethylene conversion with 34–42 wt % selectivity to the C_8^+ fraction, i.e., the jet- and diesel-range hydrocarbons, the remaining products being mainly C_4–C_8 olefins that can be recycled or valorized.[45] The resulting olefins are subsequently hydrogenated in a trickle-bed reactor packed with Pt/Al_2O_3 or Pd/C catalysts under hydrogen-rich conditions (200–350 °C, 10–40 bar), using the high-purity hydrogen produced onsite.[46] This hydrogenation step ensures full saturation of olefins into paraffins, improving fuel stability and meeting aviation specifications. The final product stream is directed to a distillation column with 25–40 theoretical stages, optimized to recover the C_8–C_{16} fraction corresponding to SPK. The SAF product obtained meets ASTM D7566 standards in terms of energy content, cold flow properties, and emissions profile. Lighter components may be recycled or valorized as LPG, while heavier fractions are suitable for diesel or lubricant blending.[47]

Figure 2 illustrates the complete process flowsheet of the proposed integrated biorefinery, which enables the coproduction of three strategic products, bioethanol, hydrogen, and SAF, within a single processing system. This configuration capitalizes on the synergistic combination of biochemical and thermochemical technologies to achieve high conversion efficiencies and minimize process redundancies. However, the primary objective of this work is to emphasize the central role of hydrogen within this system, not merely as an auxiliary reactant, but as a core product whose production, recovery,

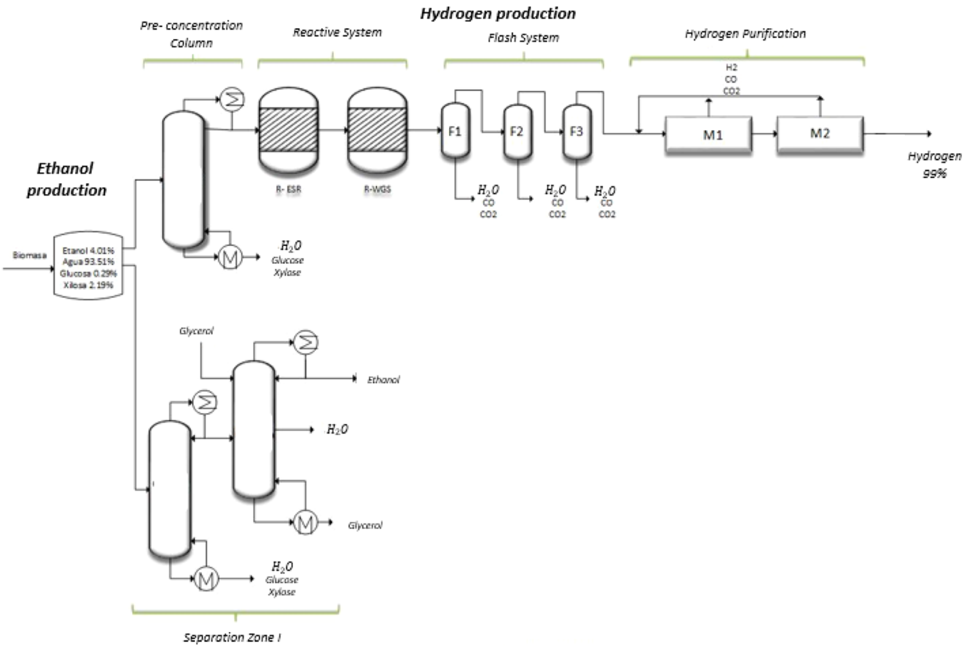

Figure 4. Simultaneous production of hydrogen and ethanol from biomass.

and integration have critical implications for the overall technical and economic performance of the biorefinery. As established in the previous sections, hydrogen is essential across various SAF production routes, particularly in the ATJ pathway, due to its function in hydrogenation and fuel quality enhancement. Within the integrated process depicted in Figure 2, two main pathways can be derived that allow hydrogen to emerge as a coproduct alongside other biobased fuels: (1) the coproduction of ethanol and hydrogen, in which part of the ethanol is diverted to steam reforming for H_2 generation, and (2) the coproduction of SAF and hydrogen, where ethanol is fully upgraded via the ATJ route while still enabling hydrogen recovery through downstream reforming or off-gas valorization strategies (see Figure 3). This manuscript is thus dedicated to the rigorous analysis and comparison of these two alternative scenarios, ethanol-hydrogen and SAF-hydrogen coproduction, to identify the most viable route for hydrogen valorization within an integrated biomass-to-jetfuel system. Both scenarios are described below.

3.2. Scenario I: Integrated Coproduction of Hydrogen and SAF

In the first evaluated scenario, an integrated process is developed to enable the simultaneous production of hydrogen and SAF within a unified biorefinery framework. This configuration aims to assess the technical, economic, and environmental feasibility of such a coproduction system and its integration potential within a bioethanol-based facility. The central feature of this scenario lies in the redistribution of purified ethanol between the ATJ pathway for SAF production and the steam reforming process for hydrogen generation.

To analyze the effect of ethanol allocation on system performance, ten operational configurations (E0 to E9) were established, each representing a different distribution ratio of ethanol between the two downstream routes. In the baseline case (E0), 100% of the ethanol is directed toward SAF production. Subsequent scenarios progressively shift ethanol from SAF to hydrogen production in 10 wt % intervals. In scenario E1, 90 wt % of ethanol is routed to SAF and 10 wt % to hydrogen, and so forth, until scenario E9, in which 90% of ethanol is dedicated to hydrogen and only 10 wt % to SAF. This systematic variation enables a comprehensive evaluation of the trade-offs between the two routes in terms of energy requirements, conversion efficiency, and economic indicators.

For hydrogen production, ethanol is initially fed into a prefractionation distillation. The concentrated ethanol stream (30 wt % ethanol/70 wt % water) is then introduced into a reforming reactor system. The gaseous output, primarily consisting of hydrogen (H_2), carbon monoxide (CO), and carbon dioxide (CO_2), is passed through a series of three flash separators to remove the residual moisture. The dry gas mixture is finally purified via a two-stage membrane separation system, where membrane surface area is scaled according to the inlet molar flow rate. This setup achieves hydrogen purity levels of approximately 99 mol %, suitable for direct use in the hydrogenation stage of the ATJ route or as a clean energy vector.

In parallel, the SAF production pathway receives the remaining ethanol fraction. This ethanol is first preconcentrated to 94 wt % in a prefractionator and then further purified to 99.5 wt % in an extractive distillation column using glycerol as an entrainer. The purified ethanol is fed into a dehydration reactor (R1) along with water, where it is converted to ethylene at 98% conversion efficiency. The reaction mixture undergoes flash separation to remove excess water and concentrate the ethylene stream, which is subsequently routed to an oligomerization reactor (R2) to produce α-olefins. These olefins are hydrogenated in reactor R3 using high-purity hydrogen produced on-site, yielding saturated paraffins and isoparaffins. The resulting hydrocarbon mixture then enters the second separation section, where light and heavy fractions are separated to recover gasoline-range hydrocarbons, SAF, diesel, and heavier oil cuts.

This scenario enables a flexible operation strategy that allows adjusting the ethanol allocation based on desired product distribution, energy demands, or market conditions. The coproduction of hydrogen and SAF in a single process thus not only improves carbon utilization but also enhances system resilience by diversifying the product slate.

3.3. Scenario II: Integrated Coproduction of Hydrogen and High-Purity Ethanol

In the second evaluated configuration, an integrated process was designed to enable the simultaneous production of hydrogen and high-purity ethanol (99.5 wt %) within a unified biorefinery system. The objective is to assess the technical and economic viability of this dual-output configuration and its integration efficiency within the broader lignocellulosic biomass-to-products framework. Figure 4 presents a schematic overview of the process and the evaluated operating scenarios.

To investigate the influence of ethanol allocation on the system's performance, ten operational scenarios were established (E0−E9). In the initial scenario (E0), the entire ethanol stream is directed toward purification, yielding 99.5 wt % ethanol. Subsequently, the ethanol feed is progressively redistributed between hydrogen and ethanol production in 10% increments. For instance, scenario E1 allocates 90% of ethanol to purification and 10% to hydrogen generation. This ratio continues until scenario E9, in which 90% of the ethanol is assigned to hydrogen production and only 10% to ethanol purification. This scenario matrix allows for a detailed analysis of the design, energy, and economic indicators associated with varying product slates.

The hydrogen production route begins with ethanol feeding into a prefractionation distillation column. The resulting stream enters the reforming system, where ethanol is converted to synthesis gas via steam reforming, followed by a water−gas shift reaction. A train of three flash separators is then employed to remove residual moisture. The dry gas stream, primarily composed of H_2, CO, and CO_2, is fed into a two-stage membrane purification unit, in which membrane surface area is tailored to the inlet molar flow. This setup achieves a hydrogen stream with a purity of 99 mol %, suitable for energy applications or chemical processes.

In parallel, the ethanol purification pathway concentrates ethanol to 94 wt % in a prefractionation column, followed by an extractive distillation column using glycerol as the entrainer to achieve 99.5 wt % ethanol purity. The two columns are designed with similar specifications, although the extractive column included solvent feed stages to enhance ethanol−water relative volatility. The resulting ethanol product complies with fuel-grade specifications and can also serve as a feedstock for chemical conversion or export.

This scenario presents a flexible platform for selectively producing hydrogen and high-purity ethanol according to process demand, market conditions, or energy strategy. By enabling the internal valorization of intermediates, this configuration enhances the overall integration, efficiency, and circularity of the biorefinery.

4. PROCESS METHODOLOGY AND PERFORMANCE EVALUATION

4.1. Process Modeling

The process was designed and simulated using Aspen Plus to evaluate the technical, economic, and environmental performance of an integrated biorefinery capable of coproducing ethanol, hydrogen, and SAF from lignocellulosic biomass. The methodology involves sequential modeling of key processing steps: ethanol production and purification, hydrogen production via steam reforming, and SAF synthesis through the ATJ pathway. Each subsystem was calibrated and validated based on literature data, and sensitivity analyses were conducted to optimize operating parameters and system integration.

In the ethanol production stage, sugar cane bagasse and corn stover were selected as feedstocks and subjected to combined steam explosion and dilute acid pretreatment to break down the lignocellulosic matrix and release fermentable sugars. Hexoses were hydrolyzed enzymatically using cellulolytic enzymes under optimized conditions (50−55 °C, 10−40 FPU/g cellulose, 30 wt % solids), while pentoses were separated as a liquor stream. Glucose-rich hydrolysates were fermented using *Saccharomyces cerevisiae*, selective to hexoses, yielding ethanol and CO_2. The fermentation broth was subsequently sent to the separation section for purification.

Regarding ethanol purification, a two-stage distillation process was modeled for ethanol recovery, comprising a prefractionation column followed by extractive distillation using glycerol as the entrainer. The NRTL thermodynamic model was employed to describe the nonideal vapor−liquid equilibrium of the ethanol−water system, which is suitable for systems exhibiting strong nonideal behavior. Each column was modeled using the RADFRAC module with a Kettle reboiler and a total condenser. Design parameters such as total stages, feed stage, reflux ratio, and column diameter were varied to achieve 99.5 wt % ethanol purity.

On the other hand, for hydrogen production, high-purity ethanol was fed into a steam reforming system followed by a WGS section. The reformer operated at 600−800 °C over a Ni-based catalyst to produce syngas. The WGS reactor, modeled at 400 °C with the Cu/ZnO catalyst, converted residual CO to additional hydrogen. Gas separation was achieved via flash drums and two polymeric membrane modules (Matrimid), yielding hydrogen with $\geq$ 99 mol % purity. The first polymer membrane module was modeled considering permeabilities of 1.3×10^{-3}, 1.54×10^{-9}, and 9.2×10^{-11} $[cm^3(Norm)cm/(cm^2s\ cmHg]$ for CO_2, H_2, and NCO, respectively. Additionally, a retentate pressure of 759.9 cmHg, a permeate pressure of 220.3 cmHg, a thickness of 0.5 cm, and a cutoff of 0.35 were considered. On the other hand, the second module was modeled with a retentate pressure of 760 cmHg, a permeate pressure of 220.4 cmHg, a thickness of 0.9 cm, and a cutoff of 0.54. In particular, previous studies by Fernández-Castro et al.[48], and Favvas et al.[49] establish clear operating pressure ranges for the type of membrane considered in this study. They claim that this type of membrane can operate with a maximum ΔP of 539.6 cmHg. Thus, considering this previously studied operating range, the operating pressure was established for permeate and retentate to allow separation according to the purity and recovery requirements.

Finally, the ATJ section was adapted from the Byogy Renewables process and modeled by using ENRTL-RK thermodynamic properties due to the presence of electrolytic species. Ethanol was first dehydrated to ethylene in an RSTOIC reactor, with 98.8% conversion. Water was removed by a series of flash units. Dry ethylene underwent oligomerization to C_8−C_{12} olefins in an RYIELD reactor, followed by hydrogenation with high-purity hydrogen in an RSTOIC reactor to produce paraffins and isoparaffins. The final product stream was separated using a RADFRAC distillation column into LPG, naphtha, SAF, diesel, and heavy oils. Operational parameters (e.g., number of stages, feed location, and reflux ratio) were tuned to maximize the jet fuel yield and comply with ASTM D7566 standards.

Each subsystem was modeled individually and then integrated into two scenarios: ethanol-hydrogen and SAF-hydrogen coproduction. A parametric study was conducted by varying the ethanol distribution across these routes (10 discrete scenarios from 100−0% to 0−100%) to assess trade-offs in yield, energy use, and economics.

4.2. Techno-Economic Evaluation

The assessment of the technological and economic viability within a sustainable development framework requires the integration of both economic profitability and environmental impact indicators. In this context, two key metrics were selected for the evaluation of the proposed biorefinery configurations: the ROI and carbon dioxide (CO_2) emissions, and minimum selling price. These parameters offer a complementary perspective on the performance of the process under study.

From an economic standpoint, the ROI and minimum selling price provide a direct measure of financial feasibility by quantifying the profitability of an investment relative to its total cost. It is widely used in industrial project evaluation to support investment decisions, particularly in emerging technologies such as biobased fuels, where capital expenditures are substantial and financial risks must be carefully managed. On the other hand, CO_2 emissions constitute a critical environmental performance metric, as climate change mitigation policies demand accurate accounting and reduction of GHG emissions across the energy value chain.

By jointly considering the ROI, minimum selling price, and CO_2 emissions, this study aims to provide a balanced and comprehensive evaluation that aligns with the principles of the circular economy, enabling the identification of optimal production scenarios with economic return and reduced environmental burden. The ROI is one of the most widely employed indicators to evaluate the economic performance of industrial processes. It is defined as the ratio between the Net Annual Profit (P) generated by the process and the Total Investment Cost (I) required for its implementation:

$$ROI = \frac{P}{I} \tag{1}$$

The net profit includes revenues from product sales minus operating and utility costs, while the total investment considers both the fixed capital investment (e.g., equipment, installation, and civil works) and the working capital necessary for continuous plant operation. In this work, the ROI was estimated using the methodology proposed in ref 50, ensuring consistency with accepted chemical process economic evaluation practices. A production configuration is considered financially viable if its ROI exceeds a minimum acceptable threshold, which typically ranges between 10−20%, depending on market conditions, risk level, and industry sector. The prices employed for SAF, ethanol, and hydrogen in this study are based on publicly available market data and recognized institutional reports to ensure transparency and relevance. Specifically, the ethanol price corresponds to the market value reported for Sweden as of July 14, 2025, amounting to USD 1.29 per liter, according to GlobalPetrolPrices.com,[51] a reputable source that provides weekly updates on international fuel prices. In the case of green hydrogen, the selected cost range is derived from estimates provided by the U.S. Energy Information Administration (EIA) and Bloomberg, as summarized in the 2021 technical report issued by the Chilean Parliamentary Technical Advisory Office.[52] This report cites production costs for green hydrogen from renewable energy sources between 3.0 and 7.5 USD/kg, while also highlighting projections of a significant cost reduction by 2030—potentially reaching values as low as 1.40 USD/kg, and further declining to 0.80 USD/kg by 2050. These figures reflect a combination of current cost assessments and forward-looking estimates based on anticipated technological improvements and reductions in renewable electricity prices. The SAF price used in the analysis follows a similar rationale, relying on market benchmarks and existing literature, although its detailed sourcing is provided in the Supporting Information of the study. Overall, the values used are consistent with credible and recent data, aiming to reflect both present conditions and plausible short-to-midterm scenarios.

On the other hand, the quantification of direct CO_2 emissions associated with process energy demands was carried out using the methodology proposed by Gadalla et al.[53] The procedure involves two steps. First, the Total Fuel Energy Requirement (Q_{fuel}) is estimated based on the reboiler duty of the process (Q_{proc}), corrected by the efficiency of the energy supply system and the heat loss in the flue gases:

$$Q_{fuel} = \frac{Q_{proc}}{\lambda_{proc}}(h_{proc} - 419)\frac{T_{FTB} - T_0}{T_{FTB} - T_{satack}} \tag{2}$$

Once Q_{fuel} is obtained, the CO_2 emissions are calculated by relating the fuel mass required to its carbon content and the stoichiometric ratio of carbon to CO_2:

$$[CO_2]_{Emiss} = \frac{Q_{fuel}}{NHV}\frac{C\%}{100}\alpha \tag{3}$$

In this analysis, butane was selected as the reference fuel due to its representative net heating value (NHV = 46,464 kJ/kg) and well-defined carbon content, making it suitable for benchmarking purposes. The resulting CO_2 emissions allow for an environmental comparison among different process configurations and support the identification of low-carbon design alternatives. For further details, please refer to the expanded model in the Supporting Information.

It is important to note that this study represents a preliminary techno-economic feasibility assessment, aiming to evaluate the comparative performance of two dual-output biorefinery configurations rather than to perform a complete plant-scale cost inventory. Accordingly, the costs associated with individual pretreatment reagents, such as acids, enzymes, and nutrients, as well as byproduct handling and waste treatment, were included implicitly within the overall operating expenditure (OPEX) factors applied in the Aspen Economic Analyzer. This level of detail is consistent with the conceptual design stage of process development, where the main objective is to identify economically promising pathways and guide further optimization. In subsequent stages of research, these aspects will be addressed through a more detailed cost inventory supported by material flow analysis and life-cycle cost assessment (LCCA), including the valorization of byproducts and environmental management of waste streams. Such a comprehensive evaluation will enable a holistic understanding of the trade-offs between economic and environmental performance in hydrogen-integrated SAF and ethanol production systems.

5. RESULTS

This section presents the results for scenarios I and II in Section 3, bearing in mind that scenario I evaluates the production of SAF and hydrogen and scenario II evaluates the production of ethanol and hydrogen.

5.1. Scenario I

As previously mentioned, biomass production and the ethanol conversion process were established as the basis of the system. The ethanol generated is divided into two streams: one destined for the hydrogen production plant and the other for the biokerosene plant via the ATJ route, maintaining the biomass-ethanol operation constant. This configuration gives rise to multiple operating scenarios, allowing for the evaluation of the technical, energy, and economic impact of different proportions of ethanol distribution between the two plants (Table 2).

As can be seen, none of the scenarios are feasible (E0−E9). The term energy balance allows us to evaluate energy production, considering that all of the fuels generated were burned, compared to the energy invested in the entire process. Therefore, it is clear that for scenario I to work a greater energy investment is required than the energy that the products themselves would release. In economic terms, the ROI reveals a poor economic scenario since none of them would generate a real profit. Although it can be seen that as the scenarios progress, the value obtained by the ROI improves, and it does not manage to exceed zero. In other words, as more ethanol is allocated to hydrogen production, the process becomes more profitable.

A similar scenario can be observed with regard to the CO_2 emissions. As economic feasibility decreases (lower ROI), CO_2 emissions increase. This behavior is understandable when considering that energy consumption is a major factor in calculating the economic feasibility of a process and that energy consumption is directly related to fuel consumption and GHG.

A potential improvement scenario involves eliminating the thermal energy demand currently associated with distillation columns. In line with emerging trends in sustainable process engineering, one promising alternative is the electrification of separation units. This strategy, which replaces traditional heat-based operations with electrically driven systems—such as high-efficiency heat pumps or electrically heated reboilers—could significantly reduce fossil fuel consumption and associated CO_2 emissions. Once the appropriate electrification infrastructure is implemented, it is expected that the energy input required by the distillation columns will no longer rely on combustion-based thermal sources. Table 3 presents the revised results under this hypothetical scenario, where the reboiler duty of the distillation columns has been completely offset through electrification, thereby allowing an evaluation of its impact on energy feasibility and economic return.

As shown in Table 3, the elimination of thermal energy consumption in the distillation columns, simulated here as a fully electrified scenario, has a noticeable impact on the system's overall energy and economic performance. In contrast to the original case, all scenarios (E0−E9) now exhibit a positive energy balance, indicating that the energy content of the products exceeds the energy input required for the process. This marks a significant improvement in energy feasibility, suggesting that electrification could be a key enabler in aligning the process with sustainability goals. From an economic

Table 2. Results of Scenarios for the Simultaneous Hydrogen and SAF Production Plant

Scenario	Total Energy Equipment (MJ)	Total Energy Final Product (MJ)	Energy Balance Q (MJ)	Equipment Q (MJ) Prefrac Column (ATJ Process)	Equipment Q (MJ) Extractive Column (ATJ Process)	Equipment Q (MJ) Separation Column (ATJ Process)	Equipment Q (MJ) Prefrac Column (H_2 Process)	Equipment Q (MJ) Prefrac Column (ATJ Process)	Capital Cost ($)	Cost of Utilities ($)	Net Profit ($)	ROI (%)	CO_2 Emission (Ton/y)
E0	1738466	1733091.8	**−5374**	863199	232781	1439	96956	0	68922789.5	973358750.4	−168900930.6	**−245**	800925
E1	2118868	1854750.8	**−264117**	777645	146209	1425	99320	550177	2257111278	980035301.1	−259118995.7	**−11.5**	1056015
E2	2002731	1734058.6	**−268673**	691232	129570	1266	86394	550177	4408208794	968969671.5	−376729414	**−8.5**	978136
E3	1899319	1575276.6	**−324043**	604819	112104	1107	87019	550177	6558085790	961589370.1	−506524589.2	**−7.7**	908790
E4	1790009	1508666.0	**−281343**	518430	99606	950	76754	550177	8707945817	965556786.3	−627365976	**−7.2**	835489
E5	1671471	1412964.3	**−258507**	432017	80742	791	63651	550177	10854340048	940241671.5	−738259146.9	**−6.8**	756000
E6	1601675	1253741.8	**−347933**	345605	64512	633	51511	595321	13000459170	933506174.2	−874357325	**−6.7**	709196
E7	1486795	1049213.9	**−437581**	259216	48765	475	38925	595321	15147440648	922841223.2	−1014611335	**−6.7**	632159
E8	1596859	1061417.4	**−535442**	172804	32840	316	25850	820956	17294394527	931696927.4	−1129920648	**−6.5**	705966
E9	1481342	873908.9	**−607433**	86409	16813	158	12914	820956	19448027840	920961423.3	−1259966989	**−6.5**	628503

Table 3. Results of Scenarios for Simultaneous Hydrogen and SAF Production without Heat Demand

Scenario	Total Energy Equipment (MJ)	Total Energy Final Product (MJ)	Energy Balance Q (MJ)	Sales Diesel ($/L) 1.32	 ATJ ($/L) 1.33	 H_2 ($/kg) 6.8	Capital Cost ($)	Cost of Utilities ($)	Net Profit ($)	ROI (%)
E0	544090	1733098	**1189008**	144008700	498437450	0	68922789.5	823515349	−93980739	**−136**
E1	544090	1854750.8	**1310661**	158220141	498774280	30514015	2257111278	826609146	−182405918	**−8.08**
E2	544090	1734058.7	**1189968**	118178514	477577989	60575219	4408208794	827858915	−306174036	**−6.95**
E3	544090	1575276.6	**1031186**	94701540	422473979	87173251	6558085790	830520796	−440990302	**−6.72**
E4	544090	1508666.1	**964576**	92265347	374749089	114604979	8707945817	832076165	−560625665	**−6.44**
E5	544090	1412964.3	**868874**	81253237	326240911	141663234	10854340048	833043784	−684660203	**−6.31**
E6	544090	1253741.8	**709652**	68512646	236956032	179368763	13000459170	834625055	−824916765	**−6.35**
E7	544090	1049213.9	**505124**	49425804	151817415	207119399	15147440648	836065732	−971223589	**−6.41**
E8	544090	1061417.5	**517327**	62394778	101416444	237483862	17294394527	838196504	$-1{,}083 \times 10^{09}$	**−6.26**
E9	544090	873909.0	**329819**	27795781	541920540	263842394	19448027840	839675704	$-1{,}219 \times 10^{09}$	**−6.27**

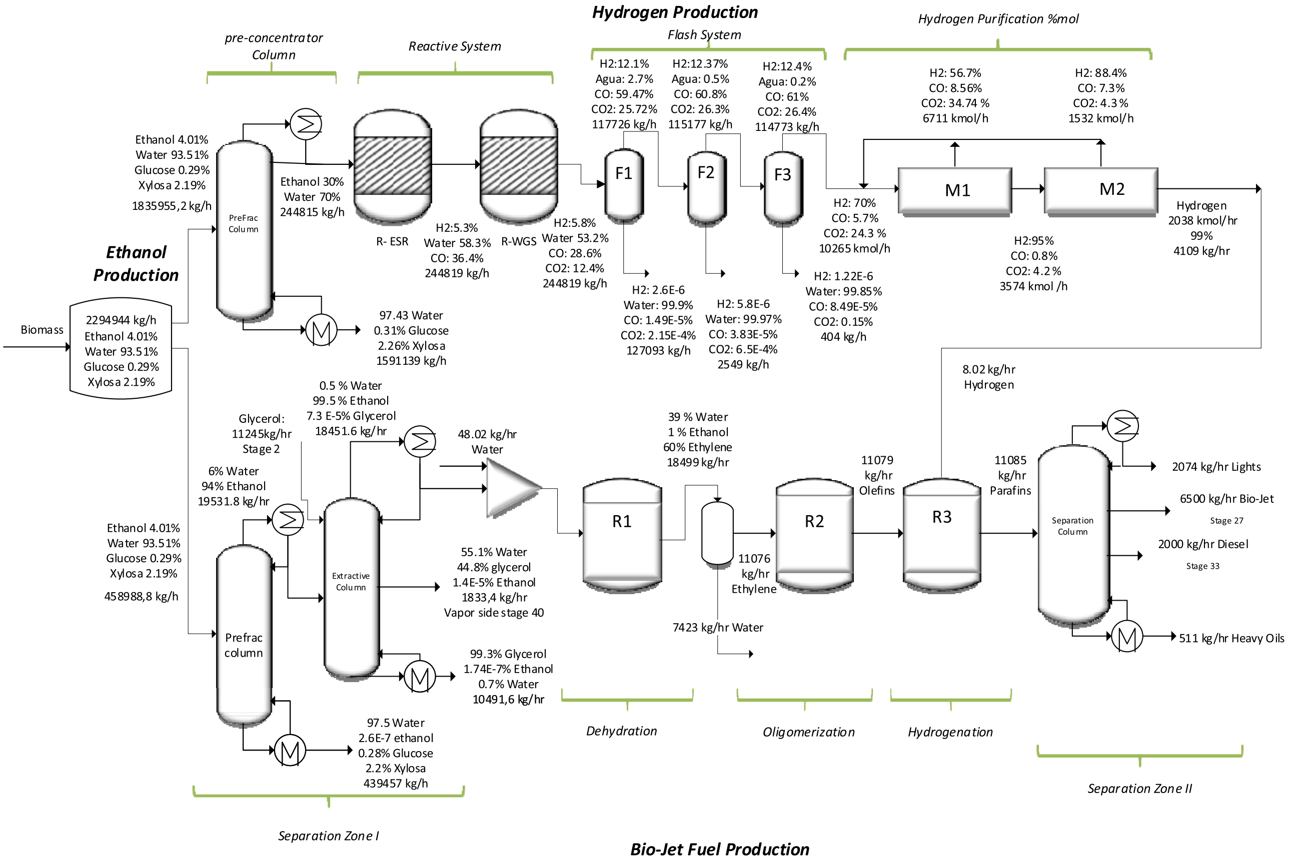

Figure 5. Mass balance for scenario E9.

perspective, while the ROI values remain below zero, they are substantially improved compared to the nonelectrified base case. For instance, scenario E1 shifts from an ROI of −11.5% to −8.08%, and scenario E5 improves from −6.8% to −6.31%. These results confirm that electrification not only reduces the environmental impact but also enhances the economic attractiveness of the process. Nonetheless, full profitability is not yet achieved, highlighting the need for further optimization or integration strategies to render the system economically viable.

While electrification of the distillation section results in a significant reduction in energy consumption and improves the overall energy balance of the system, the economic feasibility remains negative across all scenarios. This outcome can be attributed to several interrelated factors. First, although thermal energy requirements were eliminated, the process still relies on a series of complex and capital-intensive units beyond distillation, such as catalytic reactors for ethanol dehydration, oligomerization, and hydrogenation as well as advanced separation and purification systems like membrane modules for hydrogen. These units contribute substantially to both fixed investment and operating costs due to the need for specialized materials, catalysts, and utility inputs other than heat. Second, the prices assumed for the main products, 1.33 USD/L for SAF and 6.8 USD/kg for hydrogen, are not yet sufficient to offset the high capital and operational expenditures. In the absence of substantial subsidies, premium pricing mechanisms, or regulatory incentives, such as carbon credits or green fuel mandates, these product values do not generate the revenue required to achieve profitability. Addi-

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Table 4. Hydrogen and SAF Process Equipment

Equipment	P (bar)	T (°C)	Stages	Feed Stages	Reflux Ratio	Diameter (m)	Height (m)	Qreb (MW)	Length (m)	A (m)	θ
Hydrogen Process Equipment											
Pre frac column	1	100	38	15	0.79	9.8	24.94	228.4	-	-	-
ESR reactor	1.5	650	-	-	-	-	-	-	0.48	-	-
WGS reactor	1.5	400	-	-	-	-	-	-	0.7	-	-
F1	2.5	30	-	-	-	-	-	-	-	-	
F2	5	15	-	-	-	-	-	-	-	-	-
F3	10	10	-	-	-	-	-	-	-	-	-
M1	7.1	-	-	-	-	-	-	-	-	1649	0.345
M2	7.1	-	-	-	-	-	-	-	-	985.6	0.576
SAF Process Equipment											
Pre frac column	1	100	44	26	9.12	8	28.6	48.07			
Extractive column	1	78.15	60	34	0.72	1.90	35.3	9.3			
R1 reactor	13.9	369.2	-	-	-	-	-	-	-	-	-
R2 reactor	53.59	408.2	-	-	-	-	-	-	-	-	-
R3 reactor	9.01	237.3	-	-	-	-	-	-	-	-	-
Separation column	1.68	237	35	20	23.5	5.6	23.1	7.1	-	-	-

tionally, the yields of high-value products are relatively limited. Even in scenarios favoring SAF production, the multiple separation stages and the selectivity of the catalytic processes constrain the volumes of jet fuel and diesel recovered, thereby limiting income generation. Moreover, the assumption of a fully electrified setup, while beneficial for energy sustainability, implies the need for additional infrastructure and potential grid capacity upgrades, which may introduce additional hidden costs. Finally, although hydrogen is a high-value product, its production via ethanol reforming and subsequent purification remains expensive. The costs associated with catalyst consumption, reforming reactor design, and gas separation by membranes challenge the economic margin under the current market conditions, even with a selling price of 6.8 USD/kg. Figure 5, together with Table 4, shows the best solution found for scenario E8.

Based on this sale price, a natural question arises: what minimum sale price would currently be necessary for these processes to be economically feasible? Tables 5 and 6 show a picture considering only this modification for scenario E2.

Table 5. Results of Scenarios for a Simultaneous Hydrogen and SAF Production Plant with a Different Selling Price of Diesel and SAF

Scenario	Selling Prices ($) Diesel/SAF	Energy Balance (MJ)	ROI (%)
E2	2.3/2.5	−264117	**0.8**

Table 6. Results of Scenarios for Simultaneous Hydrogen and SAF Production without Heat Demand, Considering a Different Selling Price of Diesel and SAF

Scenario	Selling Prices ($) Diesel/SAF	Energy Balance (MJ)	ROI (%)
E2	2.3−2.5	1310660.6	4.2

The analysis presented in Tables 5 and 6 underscores the significant influence that product selling prices exert on the economic feasibility of integrated biorefineries. While the base case scenarios with current market prices for diesel and SAF result in negative ROI, a shift in selling prices to $2.30/L for diesel and $2.50/L for SAF leads to a considerable improvement in economic performance. Specifically, scenario E2, under these modified conditions, yields a slightly positive ROI of 0.8%, which increases to 4.2% when the process heat demand is removed through electrification. This clearly demonstrates that the financial viability of such biorefinery configurations is highly sensitive to market fluctuations and revenue streams.

Moreover, the electrification of distillation, a strategy aligned with current decarbonization trends, plays a crucial role in reducing energy inputs and improving the energy balance of the process, which, in turn, supports better economic outcomes. The synergistic effect of reduced thermal demand and higher fuel selling prices creates a scenario where integrated coproduction of SAF and hydrogen becomes a potentially feasible industrial venture.

However, it is also important to consider that global fuel markets are highly volatile and are shaped by complex geopolitical, economic, and regulatory factors. In periods of low fuel prices—such as those resulting from oversupply, shifts in energy policy, or economic recessions, this process configuration may again face economic challenges. Yet, it is precisely in such contexts that the academic and scientific value of this proposal becomes more prominent. The process design, simulation, and optimization framework developed herein can serve as a robust basis for future adaptations, policy-driven scenarios, or comparative assessments with alternative routes for biofuel and hydrogen production.

In this regard, the proposed work not only offers a pathway for sustainable fuel generation under favorable market conditions but also represents a valuable academic contribution capable of informing future techno-economic studies, guiding infrastructure planning for electrification, and supporting policy frameworks aimed at fostering resilient, circular, and low-carbon energy systems.

5.2. Scenario II

For scenario II, which considers only the simultaneous production of ethanol and hydrogen, the results in Table 7 present the obtained data.

The results obtained for Scenario II demonstrate a more favorable techno-economic performance compared to the SAF−hydrogen route. As shown in the table, scenario E1 yields a positive ROI of 3.22%, making it the only configuration among all scenarios explored in both routes that achieves economic feasibility under the current price assumptions. This outcome highlights that allocating an

Table 7. Results of Scenarios for a Simultaneous Hydrogen and Ethanol Production Plant

		Energy Requirements (MJ)			Potential Selling			
Scenario	Energy Balance Q (MJ)	Column B27	Column B12	Column B4	Ethanol (\$/L) 1.34	H_2 (\$/kg) 6.8	ROI (%)	CO2 Emissions (Ton/y)
E0	914525	863199	157473	0	1429410830	0	543	163742289
E1	1098156	777645	146209	550178	1287753400	30513776	3.22	260791005
E2	2454663	691232	129570	550178	1144672220	60574978	−2.05	219940804
E3	1643959	604819	112104	550178	1001488530	87172804	−3.86	203275994
E4	1347499	518430	99607	550178	858498470	114604684	−4.77	187411908
E5	1056209	432017	80742	550178	715415809	141662020	−5.31	170522797
E6	743268	345606	64513	595322	572334402	179353400	−5.65	161298707
E7	450461	259216	48766	595322	429252137	207071295	−5.92	144913398
E8	−63759	172804	32841	820957	286165777	236430900	−6.17	164693500
E9	−362388	86409	16813	820957	143080482	261666568	−6.32	148262342

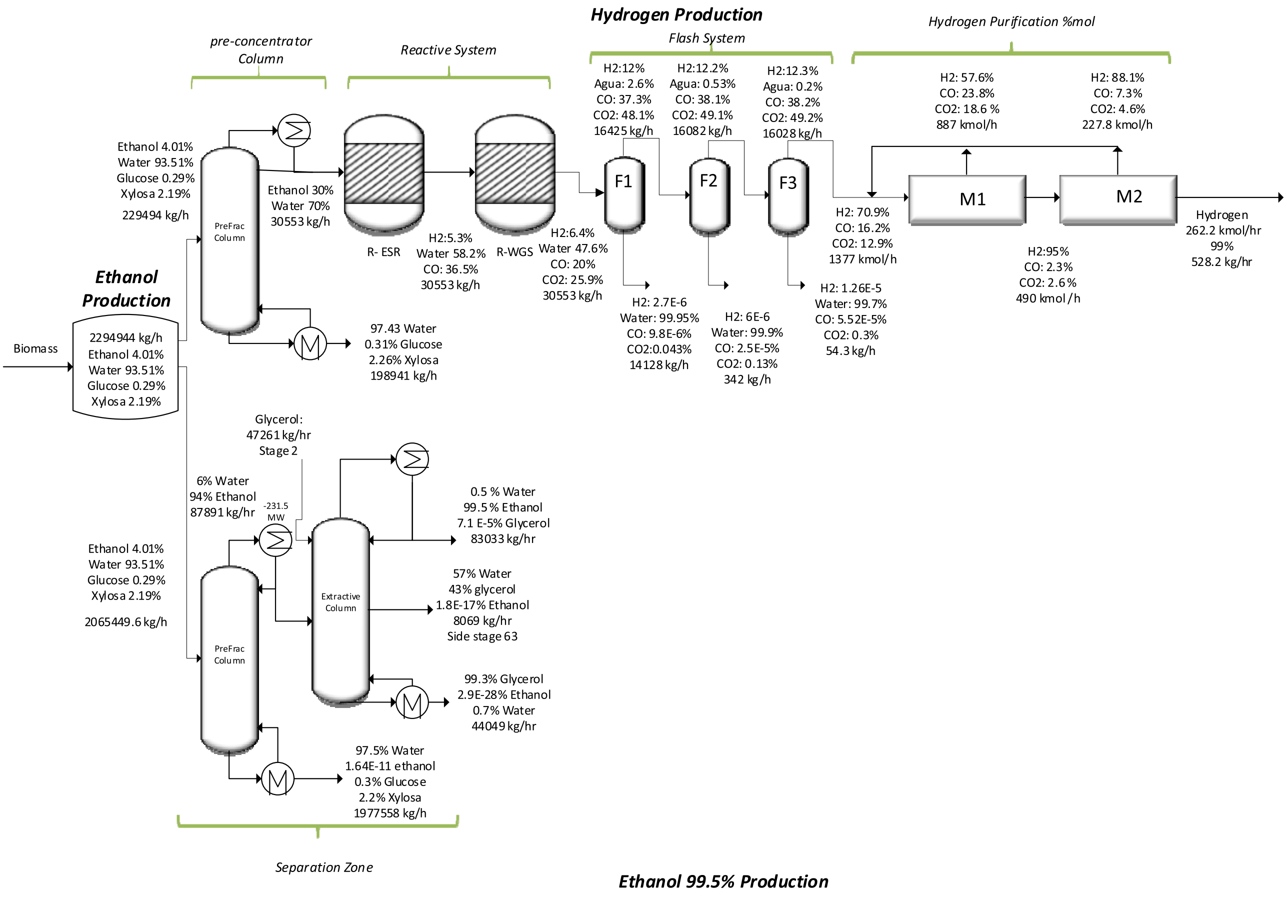

Figure 6. Mass balance for scenario E1.

optimal proportion of ethanol toward hydrogen production, while maintaining ethanol as a primary product, can significantly enhance the process profitability. Additionally, the energy balance (Q) is positive in nearly all cases, except E8 and E9, indicating that the process is generally viable from an energy standpoint. This favorable energy profile, coupled with moderate capital and operational requirements, makes the ethanol−hydrogen pathway a promising candidate for sustainable fuel production, particularly in contexts in which SAF prices remain low or uncertain.

A significant distinction between Scenario II (ethanol and hydrogen coproduction) and Scenario I (SAF and hydrogen coproduction) lies in the fact that, in Scenario II, economic feasibility is achieved without the need for additional process electrification. Specifically, scenario E1 exhibits a positive ROI of 3.22% under current market prices despite the thermal energy demands associated with distillation and reforming operations. This contrasts sharply with Scenario I, where all configurations failed to reach economic viability, unless thermal energy inputs were removed through hypothetical electrification. Moreover, the energy balance in Scenario II remains positive across nearly all scenarios (except for E8 and E9), indicating that the system is energetically robust, even under varying ethanol-to-hydrogen allocation strategies. These findings underscore the strength of the ethanol−hydrogen route as a more resilient and immediately deployable alternative, one that does not rely on infrastructure changes such as electrification to meet sustainability and profitability targets.

Table 8. Hydrogen and Ethanol High-Purity Process Equipment E1

Equipment	P (bar)	T (°C)	Stages	Feed Stages	Reflux ratio	Diameter (m)	Height (m)	Qreb (MW)	Length (m)	A (m)	θ
					Hydrogen Process Equipment						
Pre frac column	1	100	35	15	0.79	4.08	24.3	43.02	-	-	-
ESR reactor	1.5	650	-	-	-	-	-	-	0.48	-	-
WGS reactor	1.5	400	-	-	-	-	-	-	0.7	-	-
F1	2.5	30	-	-	-	-	-	-	-	-	
F2	5	15	-	-	-	-	-	-	-	-	-
F3	10	10	-	-	-	-	-	-	-	-	-
M1	7.1	-	-	-	-	-	-	-	-	4.56	0.345
M2	7.1	-	-	-	-	-	-	-	-	1.77	0.576
					Ethanol High-Purity Process Equipment						
Pre frac column	1	100	60	26	9.12	11.04	39.57	215.3	-	-	-
Extractive column	1	78.15	72	44	0.72	4.29	46.9	40.7	-	-	-

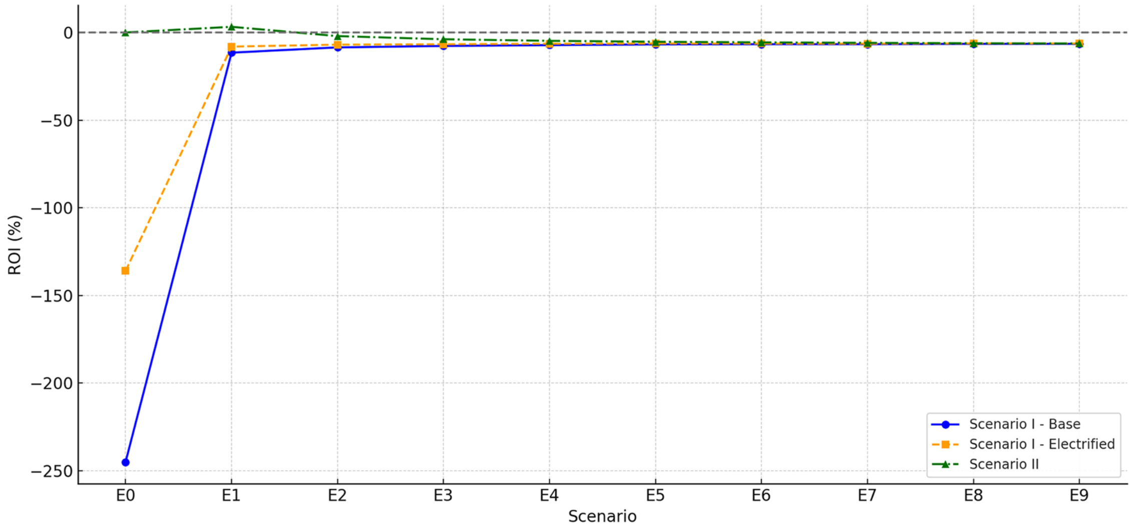

Figure 7. Return on investment for all evaluated scenarios in both configurations: Scenario I (SAF + hydrogen coproduction) and Scenario II (ethanol + hydrogen coproduction). The impact of electrification on the economic performance of Scenario I is also shown.

In a similar manner, the calculated CO_2 emissions mirror the trends observed in the economic and energy assessments. As the operational costs of the process are reduced, the return on investment (ROI) also tends to decrease, particularly in scenarios where ethanol production is prioritized over that of hydrogen. However, this cost reduction is accompanied by a corresponding decrease in process energy requirements, which directly translates into lower fuel consumption and, consequently, reduced CO_2 emissions. This inverse relationship between profitability and environmental impact highlights a trade-off inherent in the system: while higher hydrogen production improves economic performance due to its elevated market value, it also increases thermal demand and associated emissions. Conversely, favoring ethanol production moderates the energy load, allowing for a more environmentally favorable profile. This dual dynamic underscores the importance of integrated techno-economic and environmental evaluations when designing sustainable biorefinery systems.

What would happen if, as in the opposite case, there were changes in the current selling prices? Could such variations enhance the economic feasibility of the process? Exploring this possibility is essential, as fluctuations in market conditions, particularly in the value of biofuels and hydrogen, could significantly shift the profitability landscape. In scenarios in which the selling prices of ethanol or hydrogen increase beyond current levels, even modestly, the ROI could improve substantially. This suggests that under favorable economic conditions or with the implementation of supportive policies (e.g., subsidies, carbon pricing, or green premiums), the process could become not only environmentally beneficial but also economically attractive.

The results obtained for Scenario II under varying selling prices reveal important insights into the economic sensitivity and strategic potential of the ethanol−hydrogen production route. As illustrated, maintaining a constant energy balance, an increase in the hydrogen selling price from \$3/kg to \$5/kg, while keeping the ethanol price slightly adjusted from \$1.31/L to \$1.30/L, led to a marked improvement in ROI, rising from 0.8% to 2.16%. This improvement demonstrates the significant influence that hydrogen pricing exerts on the overall profitability of the system. Figure 6, together with Table 8, represents a mass balance for the best solution found.

Importantly, this scenario achieves economic feasibility without requiring process electrification or additional structural modifications, distinguishing it from Scenario I. This advantage is particularly relevant in the context of global energy transitions, where uncertainties related to fossil fuel markets and geopolitical tensions may cause fluctuations in energy prices and supply chains. In such settings, decentralized and biobased energy solutions, like the one analyzed here, become increasingly attractive not only from an economic standpoint

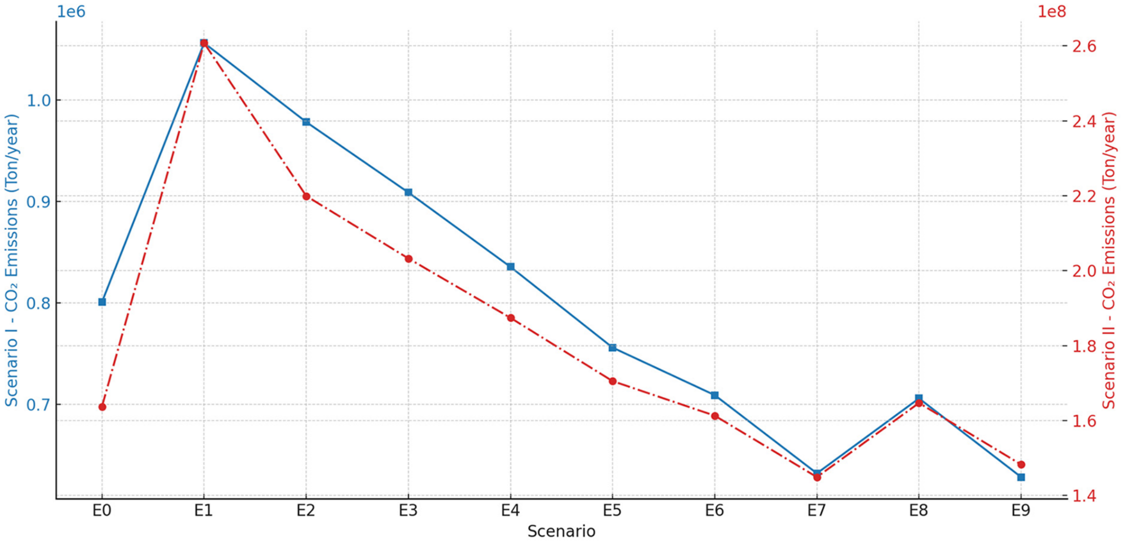

Figure 8. CO_2 emissions for all of the evaluated scenarios in both configurations. A dual *Y*-axis is used to account for the difference in emission magnitudes between Scenario I and Scenario II. This representation highlights the trade-offs between economic profitability and environmental impact under varying ethanol allocation strategies.

but also from a perspective of resilience and energy sovereignty.

To facilitate a comprehensive comparison of the performance across both configurations, Figures 7 and 8 present the results of the evaluated scenarios in terms of the Return on Investment and CO_2 emissions, respectively. These graphical representations serve to illustrate the trade-offs and trends observed when varying the ethanol distribution between hydrogen and the secondary product, either SAF or ethanol. By visualizing these key performance indicators, it becomes possible to identify configurations that offer a favorable balance between economic viability and environmental impact, thereby providing deeper insight into the systemic behavior of the integrated biorefinery alternatives.

To enhance the interpretability of the numerical results, graphical representations were incorporated to analyze the behavior of the ROI and CO_2 emissions across different operating scenarios for both configurations: Scenario I (SAF and hydrogen coproduction) and Scenario II (ethanol and hydrogen coproduction). These visualizations reveal critical insights into the trade-offs between economic performance and environmental impact under varying ethanol allocation strategies.

The ROI graph clearly demonstrates that none of the configurations in Scenario I achieve positive profitability under the current market conditions, even when electrification is introduced to reduce thermal energy consumption. While electrification leads to a marginal improvement in ROI, shifting some scenarios by up to 3%, the values remain negative across the board, underscoring the economic challenges of SAF production through the ATJ pathway. In contrast, Scenario II exhibits a more favorable economic profile, with scenario E1 achieving a positive ROI of 3.22%, which is the highest among all evaluated configurations. This confirms that prioritizing ethanol as a primary product while allocating a limited fraction to hydrogen production can lead to economic feasibility without the need for process electrification.

The behavior of the CO_2 emissions complements the economic trends. A dual-axis plot was employed to capture the different emission scales between scenarios: while Scenario I emissions range from approximately 0.6 to 1.1 million tons per year, Scenario II emissions are significantly higher, ranging from 145 to 260 million tons per year. This distinction is critical. Despite its better economic performance, Scenario II is associated with substantially greater environmental impact. The increase in hydrogen production in Scenario II, although profitable, drives up thermal energy demand and consequently, emissions. In Scenario I, the lowest ROI values (e.g., E0 and E1) coincide with the highest emission levels, and both indicators improve as more ethanol is allocated to hydrogen production. However, the absolute emissions remain considerably lower than in Scenario II.

The analysis of emissions in the study primarily focuses on the direct energy consumption associated with the process. However, it is essential to consider the indirect emissions that arise from upstream activities, which can significantly impact the overall environmental footprint. For instance, the production of catalysts used in the process involves energy-intensive manufacturing steps that can contribute to GHG. A study by the National Energy Technology Laboratory indicates that catalyst production and consumption have a minimal impact on supply chain GHG emissions compared to other stages, such as biomass preprocessing. Nonetheless, these emissions should not be overlooked in a comprehensive life-cycle assessment.[54]

Similarly, the transportation of biomass feedstocks to the processing facility entails fuel consumption and associated emissions. According to the California Air Resources Board, emissions from the collection and transportation of forest residues contribute approximately 2% of the total GHG emissions in biopower production, highlighting the importance of considering logistics in emission analyses. Incorporating these indirect emissions into the analysis provides a more holistic understanding of the environmental impacts associated with the process.[55]

Furthermore, the process aligns with the principles of circular economy and sustainability by valorizing agricultural residues into high-value energy carriers, such as ethanol and hydrogen. These outputs can substitute for fossil-derived fuels while reducing lifecycle emissions, especially when supported by policy frameworks promoting low-carbon technologies. Therefore, beyond profitability, this scenario highlights the importance of creating robust, diversified, and environmentally responsible energy portfolios that can respond flexibly to both market opportunities and global sustainability challenges.

6. CONCLUSIONS

This study assessed the technical, energy, and economic feasibility of an integrated lignocellulosic biorefinery for the coproduction of hydrogen with either SAF or ethanol. Two configurations were modeled in Aspen Plus. Scenario I (SAF + H_2) was not economically viable under current price conditions, although electrifying the distillation units significantly improved the energy balance and reduced the level of CO_2 emissions. Scenario II (ethanol + H_2) showed a more favorable performance, with one configuration (E1) achieving a positive ROI of 3.22% without requiring electrification, supported by consistently positive energy balances. Sensitivity analyses revealed that moderate increases in product prices, such as SAF at $2.5/L or hydrogen at $5/kg, could render currently unprofitable configurations viable. Environmental performance across both scenarios was strongly influenced by thermal energy demand, highlighting electrification as a key lever for reducing emissions.

The viability of implementing such systems in Mexico depends on regional biomass availability and infrastructure capacity as areas with limited feedstock or weak logistics may face higher costs and operational constraints. The results demonstrate that flexible biorefineries capable of adjusting the product distribution among ethanol, SAF, and hydrogen offer a promising pathway toward low-carbon fuel production. Future research should incorporate dynamic operation strategies, real-time market coupling, and policy-driven incentives to enhance the robustness and deployment potential of these integrated systems.

Although the proposed design methodology offers a coherent framework for assessing integrated ethanol—SAF—hydrogen biorefineries, several limitations must be acknowledged. The process simulations are based on steady-state models that do not capture dynamic behavior, feedstock fluctuations, or operational disturbances. Catalyst performance, conversion, and selectivity values were taken from the literature, and they may not fully reflect long-term deactivation. The economic analysis also relies on fixed biomass and product prices and does not consider policy incentives, such as carbon credits or SAF mandates. Likewise, the environmental assessment is limited to CO_2 emissions derived from thermal energy demand, without a full life-cycle evaluation. Despite these constraints, the methodology provides a solid foundation for determining the technical and economic feasibility of integrating hydrogen coproduction with renewable fuels. The insights obtained here help identify viable configurations and highlight the critical roles of electrification and product price dynamics. As such, this study establishes a useful baseline upon which more detailed future analyses can be built to further refine the most promising scenarios.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.5c03797.

Detailed techno-economic methodology, including Return on Investment (ROI) formulation and capital cost estimation using the Guthrie method; breakdown of fixed capital investment, working capital, and operating costs; utility cost assumptions and plant operating conditions; full economic results for all evaluated scenarios (E0−E9) for both SAF−hydrogen and ethanol−hydrogen biorefinery configurations; detailed equipment sizing and cost data; greenhouse gas (CO_2) emission calculation methodology based on process energy requirements; and supplementary tables reporting energy balances, investment costs, sales revenues, net profits, and ROI values for all scenarios (PDF)

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Notes

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■ NOMENCLATURE

GHG	Greenhouse gas
SAF	Sustainable aviation fuels
HEFA	Hydroprocessed esters and fatty acids

FT-SPK	Fischer−Tropsch synthesis
ATJ	Alcohol to jet
ICAO	International Civil Aviation Organization carbon
CORSIA	Carbon offsetting and reduction scheme for international aviation
IRA	Inflation Reduction Act
TRL	Technology readiness level
SPK	Synthetic paraffinic kerosene
SMR	Steam methane reforming
GWP	Global warming potential
WGS	Water gas shift
ROI	Return on Investment
P	Net annual profit
I	Total investment cost
EIA	Energy Information Administration
Qfuel	Total fuel energy requirement
Qproc	Reboiler duty of the process

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