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Techno-economic analysis of production of octane booster components derived from lignin

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Abstract

In this study, a comprehensive process for production of an environmentally friendly octane booster (acetophenone) from lignin is presented, along with a detailed techno-economic analysis. Recognizing that much of the prior research on octane boosters has been confined to experimental lab-level investigations, this study develops comprehensive process design to unravel the intricacies of large-scale acetophenone production. The acetophenone production process involves catalytic hydrogenolysis, which also yields phenol as a valuable side product. Based on the process flow diagram, mass and energy balances were developed, revealing significantly improved yields and purity of acetophenone compared to industry standards, reaching 0.74 kg acetophenone per kg of lignin and 99 wt%. In the techno-economic analysis, calculations involving fixed capital investment (FCI), operating costs, and working capital were conducted based on a feed of 100 kg/h of dry lignin. The results indicate FCI at 2.72 million USD, operating costs at 1.09 million USD per year, and working capital at 0.57 million USD. Assuming a 20-year operational lifespan, the payback period is estimated at 6.09 years, as depicted by the cumulative cash flow diagram. Moreover, techno-economic analysis demonstrates a net present value (NPV) of 3.24 million USD at a 10% discount rate, an internal rate of return (IRR) of 22.73%, and a return on investment (ROI) of 34.39%. These positive outcomes underscore the robust profitability of the proposed acetophenone production plant derived from lignin. Additionally, a sensitivity analysis on the IRR indicates that increasing the production capacity could further enhance profitability, reaffirming the feasibility of the plant's operation. Crucially, this study highlights the potential for sustainable and economically viable production of acetophenone, offering an environmentally friendly alternative to toxic octane boosters and advancing the development of sustainable fuel additives.

Keywords Process design · Octane booster · Techno-economic · Lignin · Biomass

Nomenclature and units

Ni	Nickel
HTC	Hydrotalcite
C_6H_6O	Phenols
C_8H_8O	Acetophenone
PSD	Pressure swing distillation
OBL	Outside battery limit
IBL	Inside battery limit
wt%	Weight percentage
FCI	Fixed capital investment
NPV	Net present value
IRR	Internal return rate
ROI	Return on investment
CCF	Cumulative cash flow
CPSPO-1	Coefficient for solid heat capacity
VSPOLY-1	Coefficient for solid molar volume of lignin

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1 Introduction

Exploration of sustainable and cost-effective alternative fuel generation technologies has recently captured worldwide interest [1]. This heightened interest is largely driven by the finite nature of oil resources, the rapidly increasing demand for oil in emerging economies, and the concerning environmental impact associated with fossil fuels. Therefore, researchers are now concentrating on alternate energy development strategies that might lessen environmental consequences, such as the development of octane boosters [2–7]. Octane booster is an additive for octane improvement of gasoline composition, which can reduce engine knocking, boost engine speeds, and thus improve overall engine performance. In the nineteenth century, however, octane boosters have had a bad reputation due to rising environmental and health concerns about both the fuel itself and the pollutants they emit from vehicles [8]. As a result, nations worldwide gradually phased out toxic octane boosters such as tetraethyl lead from the early 1970s through the mid-1990s [9]. Yet, it is critical to recognize that not all octane boosters, especially those made from biomass, should be labeled as dangerous in the same way. Simultaneously, the development of octane boosters such as biomass lignin-derived acetophenone played a critical role as a chemical additive used in gasoline to increase its octane rating.

At present, palm oil industries produce slow-degraded solid biomass waste in the form of empty fruit bunches (EFB), mesocarp fiber, palm oil mill effluent (POME), and kernel shells [10, 11]. Among them, EFB is the major solid waste, contributing 23% of palm oil industry solid waste [12]. The traditional method of dealing with palm oil waste is through mulching or burning [13]. Neither of them is effective due to the high expense of transporting waste to the mulching site and the pollutants emitted during burning waste [14]. Therefore, there is a growing scientific interest in green catalytic processes nowadays to utilize biomass in a more efficient and eco-friendly way. These techniques have a lot of appeal since they can turn biomass into profitable and high-quality products. With respect to its renewability, widespread availability in nature, and abundance, biomass stands out as a particularly attractive resource [10, 15]. This is due to the basic elements of biomass (23.7–65.0% of cellulose, 20.6–33.5% of hemicellulose, and 4.1–30.5% of lignin) [16], which have emerged as a flexible basis for numerous chemicals, industrial commodities, and biofuels [17]. Hence, biomass extracts are emerging as great possibilities for meeting growing energy demands while also presenting promising solutions to reduce environmental burdens [18]. However, most of the research today mainly focuses on sugar polymers (i.e., cellulose and hemicellulose) as they can produce glucose and xylose, which can be further produced into many products [19, 20]. Despite recent progress in the research areas for the valorization of cellulose and hemicellulose, the third main component of biomass, lignin, is still unexploited, and additional research is needed to discover its full potential.

Lignin is a complex polymer linking three basic structural elements together, including coniferyl, p-coumaryl, and sinapyl alcohol, by C—O—C and C—C linkages [21–24]. Breakage of the linkages would release aromatics and the derivatives from the lignin, which can be used to replace the fossil fuels that act as the main sources of aromatics [21]. One such possible aromatic compound that can be obtained from lignin is aromatic octane boosters [23, 25]. For instance, Shankar, Al-Abbad, El-Rachidi, Mohamed, Singh, Wang, Farooq, and Sarathy [26] investigated the potential of 2-phenyl ethanol synthesized from lignin as an octane booster. They found that the octane booster has shown promise for enhancing fuel octane quality. In addition, Tian, Van Haaren, Reijnders, and Boot [27] studied the properties of lignin-derived aromatic octane boosters, such as acetophenone, benzyl alcohol, and 2-phenyl ethanol. They concluded that all the aromatic octane boosters are non-toxic and display good knock resistance and volumetric fuel efficiency. While most research focuses on lab-scale experiments, there is a need to upscale octane booster production to an industrial level through comprehensive study, particularly for lignin-derived acetophenone.

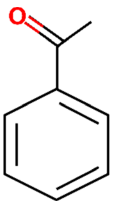
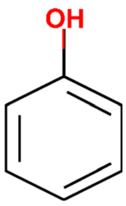
Acetophenone, a colorless and viscous liquid, has various applications as a precursor in fragrances, resins, and even as an additive to diesel fuels or a fuel for spark ignition engines [27, 28]. Notably, it stands as a safer alternative to tetraethyl lead as an octane booster due to its non-carcinogenic properties. However, the process design for producing acetophenone from bio-based lignin resources has not been clearly addressed in the literature. Traditional acetophenone production involves the liquid-phase oxidation of ethylbenzene, a process where ethylbenzene is oxidized in a solvent-free environment with the aid of a catalyst and a potent oxidizing agent [29]. Additionally, Yan, Wu, Guan, Li, Li, and Cao [30] proposed an alternative acetophenone production route through the photocatalytic oxidation of α-phenethyl alcohol using anatase and rutile titanium dioxide samples calcined at varying temperatures. While numerous researchers have explored acetophenone production from ethylbenzene, the conventional synthesis process suffers from drawbacks such as low yield, high cost, environmental pollution, significant energy consumption, and challenges in product separation, rendering it insufficient to meet the current concept of sustainable technologies [31]. Hence, exploring new and green catalytic production processes for acetophenone promises substantial economic advantages and holds great theoretical research value.

The design of catalytic systems with high selectivity for the desired product is a crucial factor in obtaining higher products. The hydrogenation of acetophenone under heterogeneous conditions has been studied with several supported monometallic catalysts. The nickel (Ni) showed an exceptionally good activity with a high conversion of over 90% towards the acetophenone, and the supported catalysts based on Ni are the most useful due to their properties and their lower cost than those based on noble metals such as Pt and Pd [32]. Hence, this paper aims to develop a comprehensive process for the production of octane booster (acetophenone) from lignin, accompanied by a thorough techno-economic analysis.

The study employs a base-case biorefinery model utilizing catalytic hydrogenolysis with nickel hydrotalcite as a catalyst and externally purchased hydrogen. The hydrogenation of acetophenone in a heterogeneous condition, employing supported catalysts based on Ni, is favored for its advantageous redox properties and cost-effectiveness, generating phenol as a byproduct [32]. Physical and chemical properties of both proposed octane boosters (acetophenone and phenol) are included in Table 1.

The results of the present study contribute to a better understanding of the potential for developing a modern bio-process to upgrade lignin into value-added chemicals, aligning with the goal of achieving net-zero objectives.

Table 1 Physical and chemical properties of acetophenone and phenol

Properties	**Acetophenone [28]**	**Phenol [33, 34]**
Molecular structure		
Chemical formula	C_8H_8O	C_6H_5OH
Family	ketone	benzene with a hydroxyl group
Molecular weight (kg/kmol)	120.15	94.11
Boiling point (K)	475.00	455.00
Density (kg/m^3)	1028.00	1058.00
Heat of vaporization (kJ/kg)	438.62	57.80
Lower heating value (MJ/L)	34.20	33.34
RON	96.1	--
MON	86.6	--
Distillation profile @P= 0.04 MPa	Heavy component	Light component
Distillation profile @P= 0.001 MPa	Light component	Heavy component
Vapor pressure, P (bar), where T = temperature (K)	log10 (P) = 4.64896 – (2006.397 / (T -43.472))	log10(P) = 4.24688 – (1509.677 / (T -98.949))

2 Methodology

2.1 Raw material and main products

2.1.1 Lignin

Lignin is nature's second most abundant biopolymer [34]. It is a complex compound with a cross-linked phenolic type of structure that is hard to break down [34]. It is more heat resistant and chemically stable than cellulose and hemicellulose due to its highly aromatic structure, resulting in an inaccurate definition of its chemical structure [34]. The study employs pure lignin as a feedstock, recovered from EFB using a sulfuric acid hydrolysis technique, followed by separation using a decanter centrifuge, as outlined in our previous work [35, 36]. The comprehensive techno-economic and environmental assessment of this lignin extraction process demonstrates its economic profitability and environmental sustainability.

2.1.2 Nickel hydrotalcite (catalyst)

Nickel (Ni) is usually employed as a base catalyst due to its lower price and abundance compared to other metals [37]. Hydrotalcite (HTC) is a type of layered double hydroxide that can be used to support Ni catalysts [37]. The structure of HTC can be defined as a plane of aluminum or magnesium atoms between two planes of the hydroxide group [25].

2.1.3 Phenol

Phenols (C_6H_6O) are organic compounds composed of an aromatic ring's carbon atom bonded to a hydroxyl group [38, 39]. They are similar to alcohols but have stronger hydrogen bonds, making them more soluble in water and less volatile than alcohols [39].

2.1.4 Acetophenone

Acetophenone (C_8H_8O) is the simplest aromatic ketone which can be naturally found in foods such as apples, apricots, bananas, cauliflower, beef, and cheese [40]. It has the sweet, pungent smell of jasmine or orange blossom and appears as a colorless liquid that is slightly soluble in water [41].

2.2 Process description

The technical and economic elements of acetophenone production from EFB-based lignin were considered. The current study calculated the production cost to estimate the profitability of acetophenone manufacturing using lignin. The simplified process flowsheet for the manufacturing of acetophenone employed in this study is shown in Fig. 1. This production consists of five major stages: catalytic hydrogenolysis, gas removal, solid separation, acetophenone and phenol purification, as well as lignin separation.

2.2.1 Catalytic hydrogenolysis

Lignin can be converted to acetophenone through catalytic hydrogenolysis (activation of hydrogen to break intermolecular bonds) [37]. In this process, a solid catalyst is preferable to a liquid catalyst as it requires a less harsh environment and does not need additional chemicals to separate the catalyst from the products [37]. The synergistic effect of Ni and HTC results in the catalytic activity of Ni-HTC, where Ni metal bonds to hydroxide ions in HTC, forming Ni

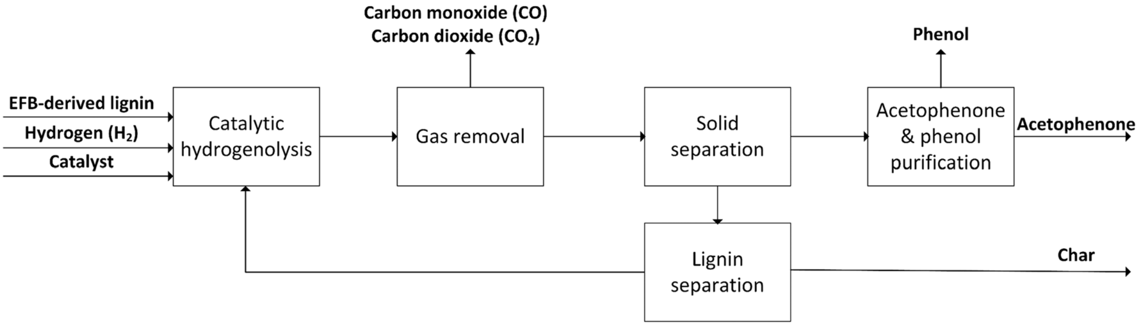


Fig. 1 Block flow diagram for production of acetophenone from lignin

hydroxide, which converts to Ni oxide upon heating (catalyst activation) [37]. This causes cleavage of β-O-4 linkage of 2-phenoxy-1-phenethanol where oxygen in the β-O-4 linkage interacts with Ni ions, which induces polymerization of the bond by weakening the C-O linkage, thus making it easy to break, resulting in products similar to those in the base catalyzed mechanism [37, 42–44]. Additionally, base catalysts also prevent the hydrogenation of aromatic rings, causing increased yield and selectivity of phenol [43].

PE is used as a representative lignin model compound since it consists of β-O-4 linkage, which is the most common linkage in lignin [37]. Catalytic hydrogenolysis of PE results in phenol and acetophenone [37]. It was found that by using a 5% Ni-HTC catalyst, a reduced metal and external hydrogen source are not needed [37]. The catalyst activity is optimum at 270 °C at this temperature, PE conversion of over 90% can be achieved [37]. However, the production of by-products such as 3.7 wt% char and less than 1 wt% carbon monoxide and dioxide is expected [43, 45].

2.2.2 Gas removal

The products of catalytic hydrogenolysis are then sent to a flash separator at 130 °C and 1 atm, where most of the phenol, with a boiling point of 181.84 °C and acetophenone, with a boiling point of 202.11 °C, will be in the liquid phase while carbon monoxide and carbon dioxide gas will be removed [46].

2.2.3 Solid separation

The remaining products will then be sent to a centrifuge to separate the liquid (acetophenone and phenol), which will be further purified, from the solid (char and unreacted lignin), some of which will be sent back to the reactor.

2.2.4 Acetophenone and phenol purification

In the liquid product, acetophenone and phenol exist as an azeotropic mixture, where they exert a binary non-ideal vapor–liquid equilibrium behavior [47]. They are classified as maximum boiling azeotropic mixtures with a maximum boiling temperature of 202.8 °C at atmospheric pressure [47, 48]. The azeotropic mixture can be separated using extractive distillation or pressure swing distillation (PSD) [47]. Both methods use two distillation columns to produce two product streams, one rich in one component while the other rich in the other [47].

Extractive distillation requires the use of a higher boiling point solvent to soak up one of the components in the azeotropic feed mixture [47]. The solvent containing one of the azeotropic components will then leave the bottom stream and go into the second distillation column, where the other azeotropic component will be recovered at the top of the column with high purity [47]. Then, in the second column, the azeotropic component in the solvent will be recovered overhead with high purity while the solvent is recycled back to the first distillation column [47]. Cumyl phenol is usually used as a solvent for the extractive distillation of acetophenone and phenol [49]. This process can produce up to 95% purity of phenol and acetophenone of up to 70% purity [49]. Since the attainable purity of acetophenone recovered from this process is only up to 70%, it might not be suitable to be used as a commercial product [49].

On the other hand, PSD uses two distillation columns with different operating pressures to separate the azeotropic mixture, so it does not require any additional chemicals to be used as a solvent [47]. This process is suitable for azeotropic mixtures that show significant azeotropic composition changes with varying operating pressure [47].

From Figs. 2 and 3, it is shown that the azeotropic composition of the acetophenone and phenol mixture changes by roughly 17% when pressure changes from 0.04 to 0.001 MPa. This suggests that PSD is suitable for the separation of acetophenone and phenol [46]. For the maximum boiling azeotropic mixture, the first column will have a higher pressure (0.04 MPa) than the second [46]. In the first distillation column, the feed composition of phenol will be higher than the azeotropic composition at 0.04 MPa (16 wt%, as shown in Fig. 2). It will be recovered as a light product at the top of the column with up to 99% purity [46]. The bottom products of the first column will have an acetophenone and phenol composition near the azeotropic composition of

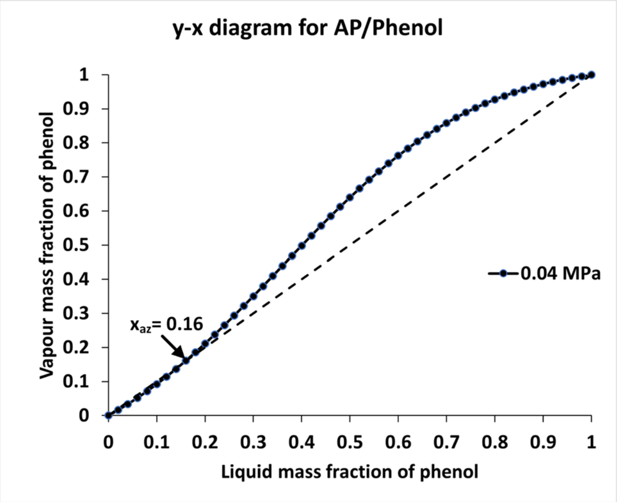


Fig. 2 *y-x* diagram of acetophenone and phenol at 0.04 MPa

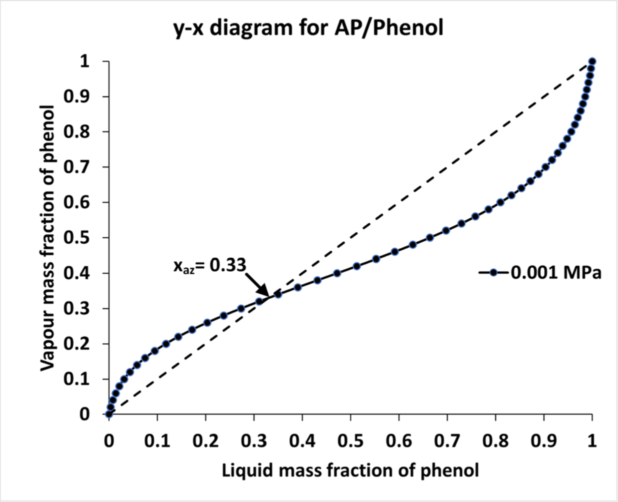


Fig. 3 *y-x* diagram of acetophenone and phenol at 0.001 MPa

0.04 MPa [47]. Since phenol is the lighter component in the bottom stream of the first column, the phenol composition in this stream will be slightly higher than its azeotropic composition at 0.04 MPa [47]. Then, the bottom stream is sent to the second distillation column with lower operating pressure (0.001 MPa) [46]. At 0.001 MPa, phenol is the heavy product since phenol composition in the bottom stream of the first column will be lower than azeotropic composition (33 wt%, as shown in Fig. 3) at 0.001 MPa. Therefore, acetophenone will be recovered as a distillate with a purity of up to 99% [46, 47]. At the bottom of the second column, since phenol is the heavy component, the phenol composition will be slightly lower than its azeotropic composition at the pressure of the second column. This stream is then recycled back to the first column [46].

2.2.5 Lignin separation

The solid products from the centrifuge will then be sent to a splitter where some of the unreacted lignin will be sent back to the reactor, and some of it will be removed along with the char.

2.3 Mass and energy balance calculation

Based on the process flow diagram (as shown in Fig. 4), and the operating conditions (as shown in Table 2), the mass and energy balances necessary for techno-economic analysis are obtained. Assumptions made are:

- The process is in a steady state.
- No pressure drops and heat loss to the surrounding (adiabatic) streams and equipment.
- Vapor–liquid equilibrium is reached in the flash separator (F1) and distillation column (PSD1 and PSD2).
- Extracted dried lignin with a particle size below 500 µm is used [50].

2.4 Techno-economic analysis

The economic model determines the fixed capital investment (FCI), operating costs, working capital, cumulative cash flow, net present value (NPV), internal rate of return (IRR), and return on investment (ROI) according to the economic assumptions. Several economic assumptions were made in the techno-economic analysis:

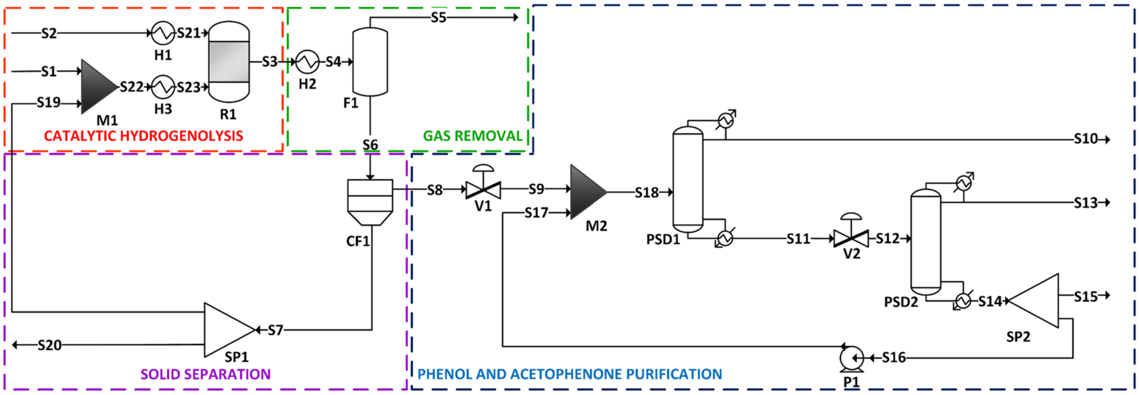


Fig. 4 Process flow diagram of acetophenone production from lignin

Table 2 Operating conditions of main equipment [38, 47]

Unit Operation	Equipment name	Operating conditions
Reaction (catalytic hydrogenolysis)	R1	270 °C 0.101 MPa
Flash	F1	130 °C 0.101 MPa
Solid liquid separation	CF1	130 °C 0.101 MPa
Distillation	PSD1	Stages: 60 0.04 MPa
Distillation	PSD2	Stages: 60 0.001 MPa

- The inventory for all raw materials, except nickel hydrotalcite catalyst, is 3 weeks.
- The inventory of nickel hydrotalcite catalyst is 5 years.
- The design and decommissioning periods of the plant are 1 year each.
- The construction period of the plant is 2 years.
- The operation period of the plant is 20 years.
- A 10% discount rate is used to calculate NPV.
- The outside battery limit (OBL) cost is 35% of the inside battery limit (IBL).
- Payroll overheads are 40% of wages.
- Maintenance labor and materials account for 2% of IBL of fixed capital, respectively.
- Insurance and property taxes are 1.5% of IBL of fixed capital.
- Book depreciation is 10% of IBL of fixed capital.
- Corporate administration is 4.5% of the total production cost.
- Research and development (R&D) accounts for 3% of the total production cost.
- Selling expenses are 10% of the total production cost.

3 Results and discussion

3.1 Mass energy balance calculations

By referring to process conditions in Sect. 2.2 and Sect. 2.3, the overall production is shown in Table 3.

Table 3 Overall result of production acetophenone from lignin

Raw materials	Lignin	Hydrogen gas
Mass flow (kg/h)	107.527	1.470
Products	Acetophenone	Phenol
Mass flow (kg/h)	48.278	50.378
Purity (wt%)	0.999	0.874

Table 4 Comparison of acetophenone production from lignin and acetophenone ethylbenzene [51]

Products/feed	Acetophenone from lignin (this study)	Acetophenone from ethylbenzene
Yield (kg product/kg feed consumed)	0.737	0.660
Purity (wt%)	0.999	0.960

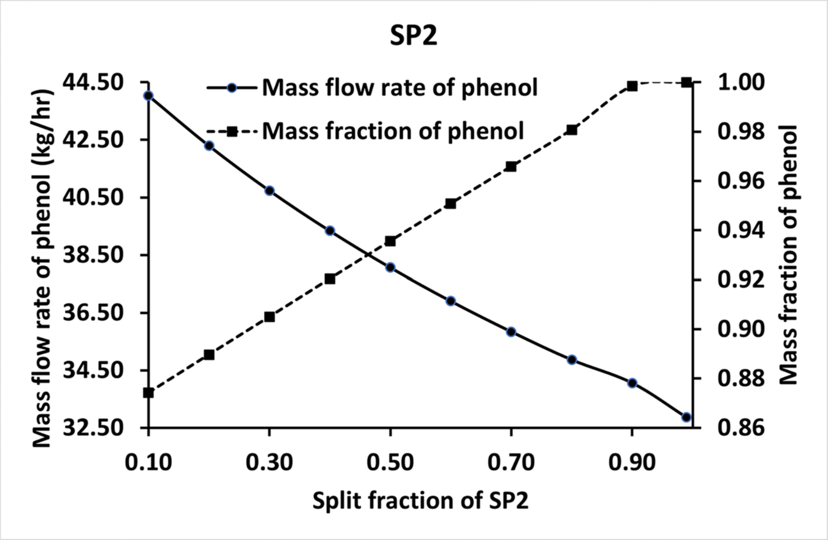
As shown in Table 4, acetophenone produced from catalytic hydrogenolysis of lignin has higher yield and purity compared to aerobic oxidation of ethylbenzene to lignin because in the former process, only one side product (phenol) is produced, while in the latter process, more side products are produced, namely, benzoic acid, benzaldehyde, phenylethyl acetate, and 2-bromoacetophenone. This causes lower acetophenone yield in the latter process due to the lower selectivity of the cobalt(II) bromide catalyst [51]. Furthermore, ether sodium bicarbonate is used to extract acetophenone from the side products of aerobic oxidation of ethylbenzene. This results in an acetophenone purity of 96%, which is slightly less efficient compared to the application of PSD, which produces acetophenone of 99.9% purity as the former process is limited by a liquid–liquid equilibrium of acetophenone and ether sodium bicarbonate [51]. Nonetheless, PSD will incur a higher capital cost due to the use of a large distillation column. This implies that the catalytic hydrogenolysis of lignin is a more efficient process for producing acetophenone compared to the aerobic oxidation of ethylbenzene, which is the current commercial process to produce acetophenone [51].

3.2 Sensitivity analyses

3.2.1 Split fraction

To increase the amount of phenol and acetophenone, a recycle stream S14 is introduced. In addition, to prevent the accumulation of products that cannot be recovered, a splitter (SP2) is added to the process. As shown in Figs. 5 and 6, the mass fraction of phenol increases with an increase in the split fraction of S15. This is because when the split fraction of S15 increases, less acetophenone from S14 is recycled back to PSD1, and the phenol recovered in S10 will have higher purity. On the other hand, the mass flow of both products (acetophenone and phenol) decreases with an increase in the split fraction of S15. This is because when the split fraction of S15 increases, less acetophenone, and phenol will be recycled back to be recovered as distillate in PSD1 and PSD2. Hence, the split fraction of S15 is minimized to maximize the flow rate of both products and ensure that some of the acetophenone is recycled back to be recovered as a product in PSD1. The split fraction of S15 to S14 is chosen to be 0.1.

Fig. 5 Mass flow and mass fraction of phenol against split fraction of S15 for SP2



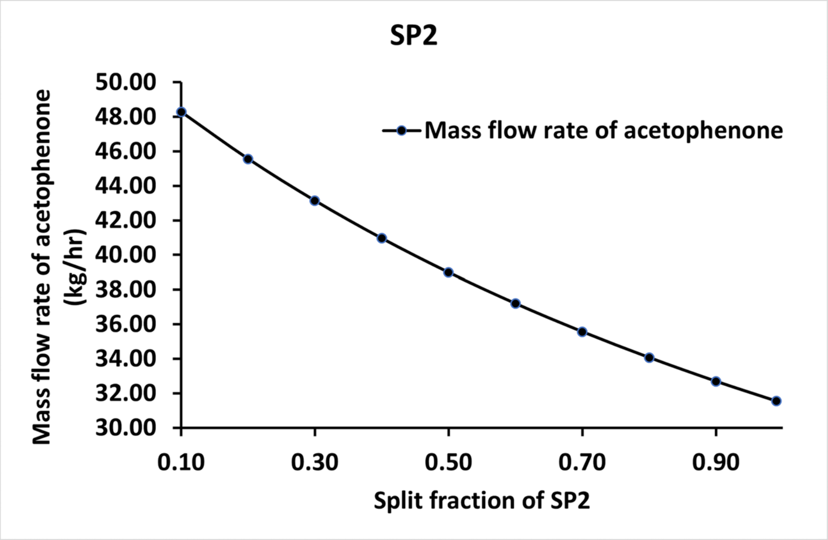
3.2.2 Pressure swing distillation pressure

The pressure in a distillation column will determine the azeotropic composition of an azeotropic mixture. As shown in Figs. 2 and 3, when the pressure of a distillation column is reduced, the azeotropic composition of the phenol mixture will increase. In a maximum boiling point mixture, the bottom product will contain a light component (phenol) with a slightly higher composition compared to the azeotropic composition and a heavy component (acetophenone) with a slightly lower composition compared to the azeotropic composition. As a result, increasing the pressure of PSD1 reduces the azeotropic composition of phenol, resulting in less phenol in the bottom stream of PSD1. Therefore, the mass fraction and mass flow of phenol recovered from the distillate stream PSD1 (S10) will increase. From Fig. 7, phenol's mass fraction and mass flow rate increase significantly with the condenser pressure of PSD1 from 0.1 to 0.4 bar. Further increases in pressure will only increase the mass fraction and mass flow rate of phenol by a little, indicating that the azeotropic composition of phenol does not have significant changes with further increases in pressure. Therefore, the condenser pressure is chosen at 0.4 bar for PSD1.

3.2.3 Pressure swing distillation mass flow ratio of distillate to feed

In PSD1, the distillate-to-feed mass flow ratio determines the mass flow of distillate (S10). As shown in Fig. 8, the mass flow rate of distillate (S10) will increase significantly with an increase in distillate to feed mass flow ratio of PSD1 until the mass flow rate ratio reaches 0.3. On the other hand,

Fig. 6 Mass flow and mass fraction of acetophenone against the split fraction of S15 for SP2



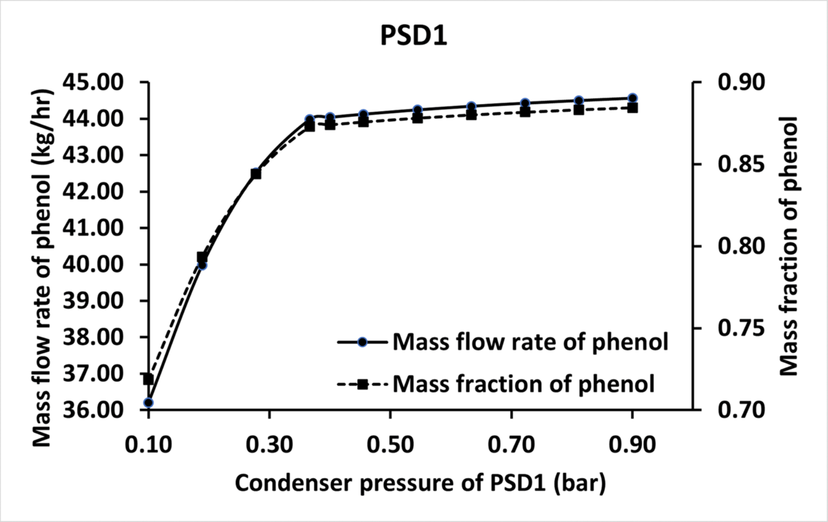


Fig. 7 Mass flow and mass fraction of phenol against condenser pressure of PSD1

the mass fraction of phenol decreases significantly with an increase in the distillate-to-feed mass flow ratio of PSD1 when the mass flow ratio is above 0.2. This is because when the distillate mass flow rate increases, more acetophenone will also be present in the distillate, thus lowering the mass fraction of phenol in the distillate. Therefore, the distillate-to-feed mass flow ratio of PSD1 is chosen as 0.313.

3.3 Techno-economic analysis results

3.3.1 Fixed capital investment

Fixed capital investment is the cost of constructing a plant. It is mainly divided into two parts: the OBL and the IBL, which can be further divided into direct and indirect costs [52]. In the direct cost, the purchased equipment cost is one of the major contributors, and other direct and indirect costs are a factor in the purchased equipment cost. Besides that, the outside battery limit is considered a factor of IBL. The calculations for equipment size and cost are shown in Appendix B.1.1 and Appendix B.1.2. This results in a total equipment cost of 476,376.22 USD, as shown in Table B.1 (see Supplementary Information, Section B), where the majority of the costs are from the distillation columns. In addition, the factors for costs are considered in fixed capital investment, and this results in total fixed capital of 2,724,205.05 USD, as shown in Table B.2 (see Supplementary Information, Section B).

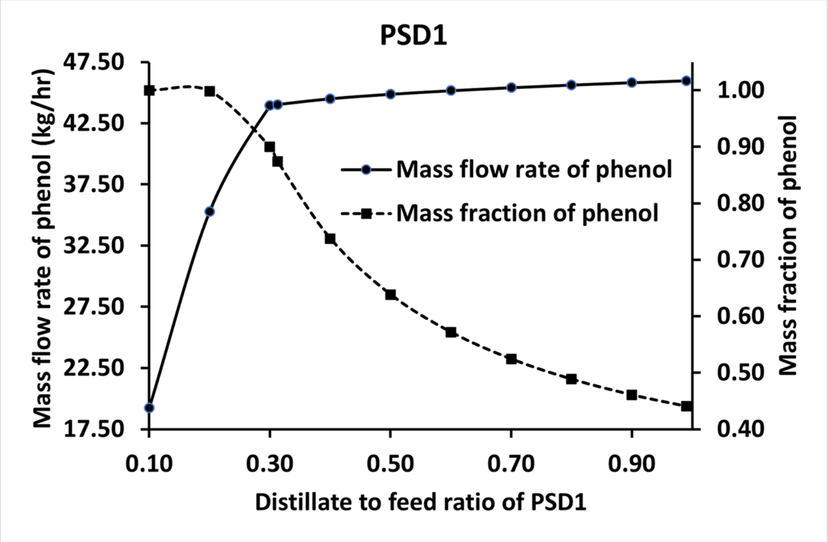
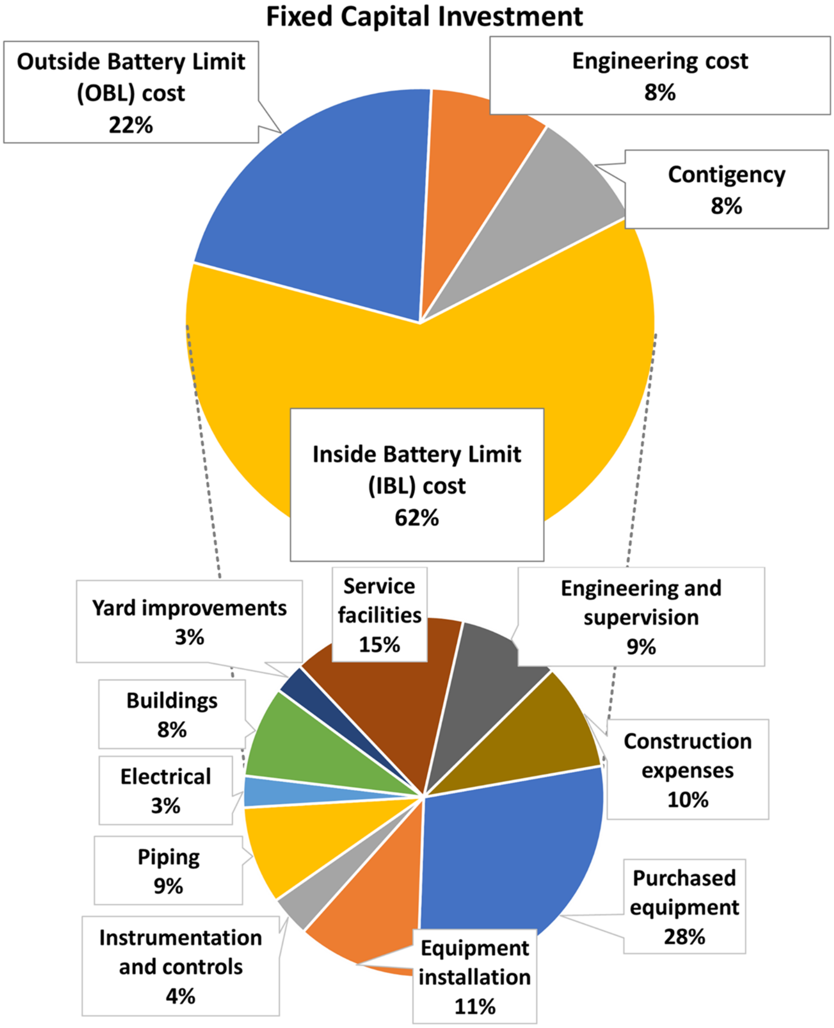


Fig. 8 Mass flow and mass fraction of phenol against mass flow rate ratio of distillate to feed in PSD1

Fig. 9 Factors considered in fixed capital investment



The percentages of costs contributing to fixed capital investment are shown in Table B.2 (see Supplementary Information, Section B). They are summarized in Fig. 9. According to Fig. 9, the fixed capital cost mainly consists of IBL, OBL, contingency, and engineering cost. IBL covers most of the fixed capital costs. IBL costs are further classified as direct and indirect, with indirect costs consisting of engineering and supervision and construction expenses and direct costs consisting of all other IBL costs (purchased equipment, equipment installation, instrumentation, and control, and so on). Most of the IBL costs are incurred due to equipment purchase.

3.3.2 Operating cost

The selling price of acetophenone (main product) and phenol (side product) is taken as 3000 USD/ton and 2000 USD/ton, respectively [53, 54]. Besides that, by knowing the raw materials and utilities needed, the operating cost of the plant can be determined. Operating costs are the daily expenses used to keep the plant running. The operating costs consist of non-manufacturing costs and manufacturing costs which can be further divided into variable and fixed costs. Appendix C.1 shows the detailed calculation for operating costs at 100% capacity utilization operating for 350 days annually. The result is then summarized in Table C.5 (see Supplementary Information, Section C), showing the total operating cost is 1.09 MUSD/y. Here, most of the operating costs are from fixed manufacturing costs, which depend on IBL, much larger than the variable manufacturing costs for this plant.

3.3.3 Working capital

Working capital is the investment of raw materials and product stock, which are important for plant operability and extended credit to clients [52]. Therefore, raw material stock, product stock, debt, and credit of the plant are considered in the working capital. For this plant, the inventory of all raw materials and products is assumed to be 3 weeks (intermittent delivery) except for the nickel hydrotalcite catalyst, which is assumed

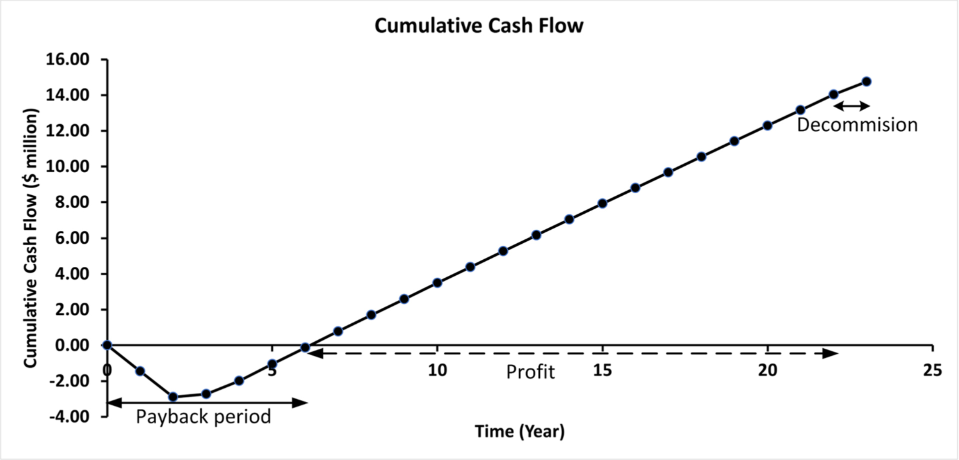


Fig. 10 Cumulative cash flow diagram for lignin to acetophenone process plant operating for 20 years

to be changed every 5 years (or 260 weeks since 1 year has 52 weeks) [52]. Besides that, all the debtors and creditors have an average indebtedness and credit period of 6 weeks, except for nickel hydrotalcite catalyst, which has a credit period of 260 weeks [52]. The total working capital is calculated as 0.57 MUSD, as shown in Table D.1, and its detailed calculation is shown in Supplementary Information (Appendix D). The account receivable (debtors) from acetophenone contributes the most to the working capital due to its high selling price.

3.3.4 Cumulative cash flow

It is assumed that the design phase of the plant will take 1 year (i.e., starting in 2022), and then the plant will be constructed within 2 years, where the fixed capital paid will be split equally within the 2 years. Furthermore, in the 2 years, 15% of working capital will be paid in year 1 and the same amount will be paid in year 2. Then, the plant will operate for 20 years, starting from year 3 (2025) until year 22 (2044). In year 3, the remaining (70%) working capital will be paid. At the start of operation (year 3), the plant is assumed to operate at 70% of the total production capacity. In the following year, year 4 (2026), the plant will increase its production capacity to 85%. After that, for the remaining operating period, the plant will operate at full capacity. Lastly, after the operating period, year 23 (2045), the plant will be decommissioned, and a salvage value of 5% is assumed, meaning 5% of total fixed capital will be recovered at this stage. In addition, 100% of the working capital will also be recovered at this stage [52].

Table E.1 (see Supplementary Information, Section E) shows the cumulative cash flow table of the plant that is then used to draw Fig. 10, the cumulative cash flow diagram of the plant. Figure 10 shows the net flow of cash into the plant over the lifespan of the project. From Fig. 10, the payback period of the plant is 6.09 years, after which the plant starts to gain profit until year 22. In the year 23, the plant will be decommissioned, where all the working capital and 5% of the fixed capital will be recovered. Figure 10 also shows that at year 23, the cumulative cash flow is 14.75 MUSD, indicating that the plant will be generating a profit.

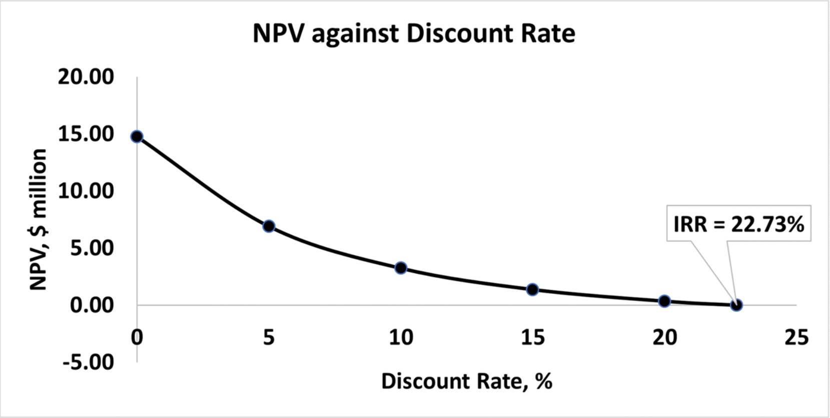


Fig. 11 NPV against discount rate

3.3.5 NPV, IRR, and ROI

Since the borrowing rates and the contribution of equity funds and loans are unclear at this stage, a discount rate of 10% can be assumed. This discount rate is used to calculate the discounted cash flow after tax of each operating year. Then the discounted cash flow of each operating year is added up to obtain the NPV of the plant, which is calculated as 3.24 MUSD as shown in Table F.1 (see Supplementary Information, Appendix F). The positive value of NPV implies net positive cash flow, indicating the project is profitable [52].

Besides that, NPV is calculated for the discount rate, and its results are shown in Fig. 11. From Fig. 11, the IRR, which is the discount rate where NPV is 0, is calculated to be 22.73%. Moreover, the ROI of the plant, which is calculated at a full production capacity of the plant, is calculated as 34.49%, and its detailed calculation is shown in Supplementary Information (Appendix F). Since the ROI calculated is more than 0%, the net income of the plant is more than its investment.

3.3.6 Sensitivity analysis

Some of the parameters in the cumulative cash flow table are varied to observe their effects on the IRR of the plant. The parameters studied are total production capacity, selling price of acetophenone and phenol, fixed capital, and variable cost. All the parameters are decreased (negative variation) and then increased (positive variation) by 10%.

Figure 12 shows that the total production capacity of a plant has the most significant effect on IRR. A 10% increase in total production capacity leads to an IRR increase of the plant by 15.76% of its original value. Besides that, the selling price of acetophenone, fixed capital, and selling price of phenol also have a significant effect on the IRR of the plant. Thus, if the selling price of acetophenone and phenol decreases or fixed capital increases, the total production capacity of the plant needs to be increased to maintain or improve profit. Lastly, the variable cost has the least effect on IRR due to less amount of utility used and the low price of raw material (lignin).

3.4 Plant viability

Section 3.3.5 shows positive NPV, IRR, and ROI for a plant producing acetophenone from lignin. Hence, it will be a profitable process plant. This is the result of using lignin as the raw material to produce acetophenone. Lignin is the by-product of the palm oil industry, which is produced in abundance in Malaysia. It is often considered a waste, and the common disposal methods are using it as mulch or burning it as fuel. Therefore, it is sold as cheap biomass, resulting in a lower operating cost.

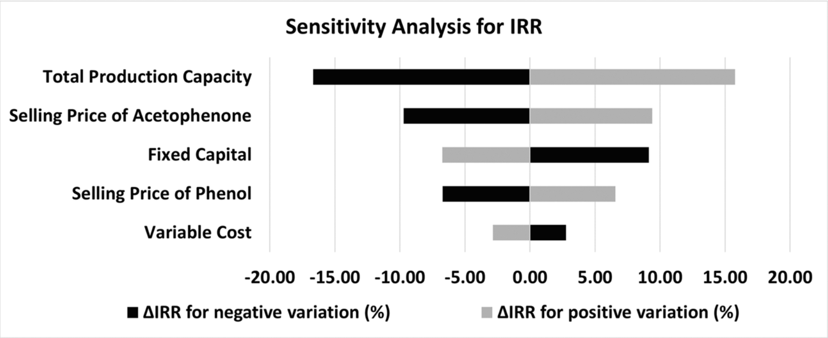
Due to the rising demand in the pharmaceutical, cosmetic, and other industries using acetophenone and phenol derivatives as raw materials, the demand for acetophenone and phenol is also expected to rise in the coming years [40, 55]. Consequently, the selling price of acetophenone and phenol is expected to stay or rise, and the total production capacity of the plant can be increased to increase profit.

3.5 Limitation and future recommendation

The assumption of a steady-state operation in this study may oversimplify the dynamic system behavior of acetophenone production, lacking the ability to adequately represent transient conditions and dynamic responses to operational changes. Notably, this assumes successful catalytic hydrogenolysis to produce acetophenone, with kinetics reactions depending on the specific catalyst used and data obtained from literature. Furthermore, the techno-economic sensitivity analysis does not include the significant risk factors such as fluctuations in product yields, which are common in pioneer plants.

Enhancing model accuracy in future improvements requires consideration of artificial neural network models, detailed kinetic models, and risk factors related to product yield fluctuations. In future, the development of lignin-derived octane boosters will need an in-depth evaluation of various critical aspects such as the business outlook, environmental concerns, social implications, and governmental legislation. Strategic business initiatives involve the identification of targeted markets and the

Fig. 12 Sensitivity analysis of IRR



establishment of industry collaborations, improving manufacturing processes and promoting competitiveness. Additionally, adopting a system dynamic approach with a quantitative focus is proposed to ensure a more reliable cause-and-effect analysis, particularly concerning policy making. This approach allows for a detailed exploration of potential scenarios, including the impact of increased AP cost on society. Besides, the implementation of a social life cycle assessment is proposed, aiming to comprehensively evaluate the environmental and societal impacts extending from lignin extraction to acetophenone (AP) utilization, thereby fostering a holistic understanding of sustainability. Lastly, government involvement is crucial, with potential measures including the provision of incentives, subsidies, and supportive regulations to incentivize the adoption of AP and facilitate their integration into the market.

4 Conclusion

In this study, a process design to produce an alternative "greener" octane booster (i.e., acetophenone) from lignin is proposed followed by a comprehensive techno-economic analysis. Catalytic hydrogenolysis is employed to produce acetophenone, with phenol as a by-product. The study reveals superior yields (0.74 kg acetophenone/kg lignin) and purity (99 wt%) compared to existing market standards. Economic evaluations, based on a feed of 100 kg/h dry lignin, showcase a robust investment with a fixed capital investment (FCI) of 2.72 MUSD, operating costs of 1.09 MUSD/year, and a payback period of 6.09 years over a 20-year operational lifespan. Techno-economic analysis yields a net present value (NPV) of 3.24 MUSD, an internal rate of return (IRR) of 22.73%, and a return on investment (ROI) of 34.39%. Therefore, those positive results prove that the proposed acetophenone production plant derived from lignin is robust and profitable. Finally, a sensitivity analysis was performed on the IRR, and the results revealed that the total production capacity of the process plant could be increased to further increase profit, proving the feasibility of the plant. In terms of the practical implication, this study promotes substituting environmentally harmful octane boosters with sustainable acetophenone from lignin, urging policy changes and regulations to endorse environmentally sustainable octane boosters. It illustrates the economic potential of lignin valorization as a valuable resource for investors, seeking support for environmentally friendly octane booster initiatives. The significant impact of environmentally friendly acetophenone extends beyond academia, guiding policymakers and investors towards sustainable practices, aligning with broader environmental goals for a greener and economically viable fuel industry.

Future development of lignin-derived octane boosters requires an in-depth evaluation covering business, environmental, social, and legislative aspects. Market identification, industry alliances, process improvements, and competitiveness promotion are all part of strategic efforts. A system dynamic approach with a quantitative emphasis facilitates reliable cause-and-effect analysis, taking into account conceivable situations such as the societal effects of rising acetophenone prices. Implementing a social life cycle assessment also ensures comprehensive evaluation from lignin extraction to acetophenone utilization, fostering a holistic understanding of sustainability. Government involvement is critical, with recommended measures such as incentives, subsidies, and supportive regulations to encourage acetophenone usage and facilitate market integration. These collective efforts will drive the transition towards a more environmentally sustainable and economically viable future in the fuel industry.

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Data Availability Data will be made available upon reasonable request.

Declarations

Ethical approval Not applicable.

Competing interests The authors declare no competing interests.

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