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ORIGINAL RESEARCH PAPER

Optimized Sustainable Production of Catechol from Lignin-Rich Agricultural Waste

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Abstract
This study addresses critical challenges in the chemical industry, including resource depletion, energy consumption, and environmental impact, by investigating sustainable and economically feasible processes for catechol production from corn stover. Using the Differential Evolution with Tabu List (DETL) methodology, this research aims to optimize the production process by minimizing environmental indicators and maximizing Return on Investment (ROI) and the Inherent Safety Index (ISI). Two pretreatment methods—dilute acid and organosolv—are evaluated to assess their efficiency in converting lignin-rich biomass into catechol. The optimization process revealed several designs achieving high catechol purity of 98%, with recovery rates up to 390% higher for the organosolv method compared to the dilute acid method. The ROI for the organosolv method was found to be 41%, in contrast to 33% for the dilute acid method, while the environmental impact of organosolv (1.11×10^8 pts/kg catechol) was higher than that of dilute acid (4.06×10^6 pts/kg catechol). Through the integration of advanced optimization tools, the study proposes two sustainable designs for catechol production, underscoring the significance of selecting appropriate pretreatment methods. These findings support the goals of green chemistry and the United Nations' 2030 Agenda, enhancing the valorization of agricultural waste and fostering more sustainable industrial practices. This research sets a precedent for future innovations in the biorefinery sector, demonstrating the potential of advanced methodologies to develop efficient and environmentally responsible chemical processes.

Keywords Catechol production · Corn stover · Lignin-rich biomass · Stochastic optimization · Biorefinery sustainability

Nomenclatures

C_i	Impact value for category i
$P_{x,y}$	Impact probability
f_i	Frequency of occurrence
$\sum$	Summation
I	Total investment
Min	Minimize
NRTL	Non-random two-liquid model
P	Net profit
ROI	Return on Investment
x,y,z	Decision variables
$EI99$	Eco-Indicator 99
IR	Inherent Safety Index
α	Quantity being evaluated
ω	Weighting factor for damage

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Introduction

Sustainability is a central theme in the twenty-first century due to concerns over climate change and excessive resource use. As the global population grows, the demand for natural resources intensifies, making sustainable practices crucial. Sustainability balances economic development, environmental protection, and social responsibility, ensuring the well-being of present and future generations (Jindal et al. 2023). The international community adopted the 2030 Agenda for Sustainable Development, aiming for development in economic, social, and environmental dimensions all while helping climate change. A key aspect of the 2030 Agenda is promoting the sustainable use of natural resources and adopting responsible production and consumption practices. The valorization of lignocellulosic biomass emerges as a promising strategy. This biomass includes plant materials such as wood, agricultural residues, and forestry waste, which are abundant and renewable carbon sources that can be converted into high-value chemicals and materials (Segovia-Hernández et al., 2023).

Lignocellulosic biomass is composed of cellulose, hemicellulose, and lignin (Stefanidis et al. 2014). Cellulose and hemicellulose have been extensively studied and valorized into chemicals like bioethanol, bioplastics, and other bio-based chemicals (Kaur & Kaur 2021). Being cellulose, the most abundant organic polymer used in various industrial applications, while hemicellulose has significant potential for producing biofuels and renewable chemicals (Rosini et al. 2023). Biorefineries present a sustainable strategy for valorizing lignocellulosic biomass. Similar to petroleum refineries, biorefineries convert lignocellulosic biomass into chemicals, biofuels, and high-value materials. They integrate multiple processes and technologies to maximize biomass utilization, minimize waste, and reduce environmental impact (Chettri et al. 2023). Modern biorefineries process various lignocellulosic feedstocks through biochemical, thermochemical, and chemical processes. Biochemical processes, such as fermentation and anaerobic digestion, use microorganisms and enzymes to break down biomass into simple sugars and compounds, which are converted into biofuels and chemicals. Thermochemical processes, like pyrolysis and gasification, use heat and chemicals to decompose biomass into gases and liquids refined into various products. Chemical processes, such as hydrolysis and transesterification, transform biomass components into valuable chemicals (Martínková et al. 2023).

Integrating these processes within a biorefinery allows for efficient production of a wide range of products, from biofuels and bioplastics to high value chemicals and advanced materials. Additionally, biorefineries leverage by-products and residues, converting them into useful products and minimizing waste. This makes biorefineries a promising solution for promoting sustainability and reducing dependence on fossil resources. Besides environmental benefits, biorefineries offer economic and social advantages. They can boost economic development in rural areas, provide employment, and promote innovation and technological development, enhancing industry competitiveness and creating new business opportunities (Wang et al. 2023).

Lignin, on the other hand, consists of polyaromatic oxygenated compounds and presents significant challenges for conversion into biofuels due to its stable and nonreactive aromatic structure (Suresh et al. 2021). This stability makes it difficult to process lignin effectively, leading to the production of large amounts of coke when using certain catalysts, such as ZSM-5 (Qian et al. 2021). Despite these challenges, lignin can be converted into valuable products. For instance, it can be processed to produce gasoline, olefins, and light cycle oil through catalytic cracking. However, the yields of liquid products from lignin processing can be relatively low, and the process often results in substantial coke and char formation, which complicates the overall conversion efficiency (Li et al. 2015). Overall, while lignin has potential as a feedstock for biofuels, its recalcitrant nature and the challenges associated with its conversion remain significant hurdles (Huber and Corma 2007).

Lignin is a recalcitrant compound that poses challenges for valorization, and there are still opportunities to generate high-value organic compounds from it (Chen & Wan 2017). Specifically, it has the potential to produce benzene from catechol in such a way that lignin can be transformed into valuable aromatic compounds through appropriate chemical processes. Lignin can be transformed into various products, including C7–C11 alkylbenzenes and multi-branched paraffins through hydrotreating and catalytic cracking processes. These processes can yield high-value compounds, suggesting that there is potential for developing biorefineries that utilize lignin as a feedstock to produce valuable organic chemicals and fuels (Carceller et al. 2024).

Catechol, a high-value compound, is used in the chemical, pharmaceutical, and materials industries (Shorey et al. 2024; Zhan et al. 2023). The valorization of lignin into catechol enhances the value of lignocellulosic biomass and promotes sustainability. Efficient conversion requires advanced technologies and catalytic processes. Research includes metal catalysts, biological processes, and chemical depolymerization techniques. Few cases in literature optimize lignin valorization processes. Mabrouk et al. (2018) conducted an exergy and economic study for producing catechol from lignin derived from olive pruning waste. The plant, with a capacity of 2544 kg/day, involves delignification to separate fibers, depolymerization to convert lignin into catechol, and a series of separation columns for catechol recovery. However, the process is not optimized, leading to inefficiencies and higher costs. Designing a biorefinery to valorize lignin into catechol is relevant for diversifying and adding value to lignocellulosic biomass. Catechol, with its industrial applications, can become a central product, enhancing economic viability and reducing dependence on fossil sources (Guo et al. 2024). Lignin valorization within a biorefinery mitigates environmental issues associated with lignocellulosic waste disposal. Transforming lignin into valuable chemicals promotes a circular economy, reducing carbon emissions from biomass burning and landfill pressure (Wu et al. 2023).

This work aims to design a biorefinery for catechol production from lignin, optimizing the process within a sustainability framework using economic, environmental, and safety indicators. Advanced modeling and simulation tools will evaluate process configurations and optimization techniques. The Eco-indicator 99 (EI99) method will assess environmental impact, and economic analysis will focus on costs. Safety analysis will identify hazards and propose risk mitigation measures. The goal is to develop a robust, sustainable biorefinery process that serves as a model for future lignin-based biorefineries. Successful implementation could advance bio-based chemicals, providing an alternative to petrochemical routes and supporting a sustainable industrial paradigm.

Problem Statement

The chemical industry is currently facing significant challenges related to resource depletion, energy consumption, and environmental impact. To address these issues, there is an urgent need to develop sustainable and efficient processes. Traditional practices in the industry have led to considerable environmental damage, including greenhouse gas emissions and pollution of water and soils. Consequently, finding alternatives to reduce these emissions and manage waste more effectively is critical. One promising approach involves the utilization of agro-industrial waste, which is abundantly available. Globally, approximately 200 billion tons of agro-industrial waste are produced annually (Mankar et al. 2021). In Mexico, around 25% of harvested agricultural products result in waste (corn, rice, sorghum, etc.) amounting to approximately 268.9 million tons of agricultural solid waste each year (Gutiérrez et al., 2020).

Currently, a significant portion of this waste is either burned or improperly disposed of, leading to severe environmental consequences. Agricultural burning, for instance, contributes to air, soil, and water pollution and releases harmful gases like CO_2, N_2O, and hydrocarbons into the atmosphere, with 1.7×10^{13} particles of harmful gases emitted per kilogram of burned corn stover (Satyendra et al. 2013). This practice also reduces soil fertility and water retention capacity by 25–30%, necessitating costly and environmentally harmful interventions (UN 2020). Given the substantial environmental impact of current waste disposal practices, there is a growing interest in transforming agricultural waste into economically valuable products. Lignocellulosic biomass, particularly from corn stover, presents a viable alternative due to its abundance and potential for conversion into high-value products such as catechol. Corn stover is one of the most abundant biomass residues in Mexico, with an availability of approximately 48.2 million tons per year (Contreras-Zarazúa et al. 2022).

Despite the high potential, the revalorization of lignin from biomass for catechol production remains underexplored at an industrial scale. Currently, only about 2% of lignin is utilized for producing high-value chemicals, such as catechol, which is primarily used in pharmaceuticals, agrochemicals, and polymer industries (Montazeri & Eckelman 2016). Moreover, there is no recorded industrial design for valorizing biomass through lignin conversion to catechol that incorporates optimization tools considering sustainability, economic feasibility, and safety. Lignocellulosic biomass is composed of cellulose, hemicellulose, and lignin. Processes that utilize biomass often discard lignin during pre-treatment, which separates the biomass into its constituent components. Lignin, however, represents a valuable raw material that can be converted into high-value chemicals like catechol. Therefore, the primary objective of this study is to design and optimize a sustainable, economically viable, and environmentally friendly process for converting lignin from corn stover into catechol. This involves selecting appropriate pre-treatment methods, modeling the conversion process, and optimizing the design using sustainability metrics such as the EI99, ROI, and IR. By addressing these aspects, the study aims to demonstrate the feasibility of transforming agricultural waste into valuable bioproducts, contributing to the principles of green chemistry and the United Nations' 2030 Agenda for Sustainable Development.

Methodology

Process Description

The study aims to optimize the production of catechol from corn stover using lignin-rich biomass. The process involves two pretreatment methods: dilute acid and organosolv. The goal is to achieve high-purity catechol with minimized environmental impact and maximized ROI. The optimization process uses the DETL methodology.

The dilute acid pretreatment process begins with mixing corn stover with water and sulfuric acid. This mixture is heated to 158 °C and then enters the pretreatment reactor where cellulose and hemicellulose are degraded into xylose and glucose. Xylose is further dehydrated to furfural. After these reactions, the mixture is filtered to separate solids and liquids. The liquid phase is neutralized to convert the acid into a neutral compound, and lignin is isolated from the mixture. The isolated lignin undergoes further reactions to produce catechol, followed by purification processes to achieve high-purity catechol.

In the organosolv pretreatment process, corn stover is mixed with water and ethanol and heated to 180 °C. The mixture enters the pretreatment reactor where partial delignification occurs using organic solvents. The mixture undergoes washing to recover solvents and distillation to separate components. Lignin is isolated from the mixture and then converted into catechol through specific chemical reactions and purification processes to achieve high-purity catechol.

Both processes include separation and purification steps. Following the pretreatment, the solid and liquid phases are separated. The liquid phase is processed in a flash tank to remove volatile compounds. The isolated lignin undergoes chemical reactions to produce catechol, and the final mixture is distilled to separate catechol from other by-products, achieving the desired purity level (see Figs. 1 and 2).

Process Modeling

The simulation of the process was carried out using Aspen Plus version 12. The process design was modeled from scratch, selecting the most suitable pretreatments to achieve maximum lignin purity. The simulation included mass and energy balances, reaction kinetics, and thermodynamic properties. The feedstock considered was 4057.09 kg/h of corn stover biomass for both treatments, representing 0.1% of the daily agricultural residues in Guanajuato.

The feedstock used for the simulation is a lignin-rich biomass composed of 44.38% cellulose, 33.63% hemicellulose, and 21.99% lignin, consistent with typical values reported for agricultural residues (Contreras-Zarazúa et al. 2022). As shown in Table 1, the compositions used in the simulation are representative of different types of agricultural residue biomass. Similar biomass compositions have also been employed in other studies for the production of bioproducts (Woo et al. 2023). The high lignin content supports catechol production, while cellulose and hemicellulose enhance processing characteristics during pretreatment. These values ensure the accuracy and reproducibility of the simulation results.

The non-random two-liquid (NRTL) model was used for the thermodynamic calculations, following the Carlson algorithm as detailed by Carlson (1996). The NRTL model is justified due to its ability to accurately predict the phase behavior of non-ideal mixtures, which is essential for the complex mixtures involved in the biomass conversion process.

Dilute Acid Pretreatment Process Design

The first step is the acid pretreatment where water and sulfuric acid are mixed and heated to 158 °C before entering the pretreatment reactor with corn stover. The proportions were 78% water and 12% biomass. The main reactions and their conversions are shown in Table 2.

The mixture then undergoes filtration, and the liquid phase enters a flash tank while the solid and liquid phases move to a neutralization reactor, as shown below (Table 3).

After neutralization, the mixture is filtered to separate calcium sulfate, followed by reactions in the cellulose and glucose reactors as detailed in Tables 4 and 5.

The lignin solution then undergoes catechol production in the final reactor as shown in Table 6.

The complete process design for acid pretreatment is shown in Fig. 1.

Organosolv Pretreatment Process Design

For the organosolv process, 78% water, 12% biomass, and 24% ethanol are mixed and heated to 180 °C before entering the pretreatment reactor. The main reactions and their conversions are shown in Table 7**.**

The process continues with filtration, washing, and solvent recovery. The lignin solution then undergoes catechol production in the final reactor as shown in Table 8.

The complete process design for organosolv pretreatment is shown in Fig. 2.

Process Assesment

In the pursuit of sustainable industrial practices, the evaluation of chemical processes requires a comprehensive assessment that balances economic viability, environmental impact, and safety. This study employs three critical indices—ROI, EI99, and IR—to evaluate the catechol production process from lignin-rich biomass. ROI measures the economic feasibility, ensuring that the process is financially sustainable and attractive for industrial implementation. The EI99 provides a quantitative assessment of the environmental impact, aligning with the SDGs that aim to mitigate climate change and reduce ecological footprints. Finally, the Inherent Safety Index assesses the process's safety, a crucial factor in reducing risks to workers and communities, thereby supporting the goal of fostering safe and inclusive working environments. Together, these indices offer a holistic evaluation framework that not only ensures the process's efficiency and profitability but also its alignment with the broader objectives of the UN's 2030 Agenda for Sustainable Development. By integrating these indices, the study emphasizes the importance of developing chemical processes that are economically sound, environmentally responsible, and inherently safe.

Thus, performance indicators were based on sustainability concepts, including economic, environmental, and safety metrics.

Economic Indicator: ROI

The Return on Investment (ROI) is a critical metric for evaluating the economic performance of the catechol production

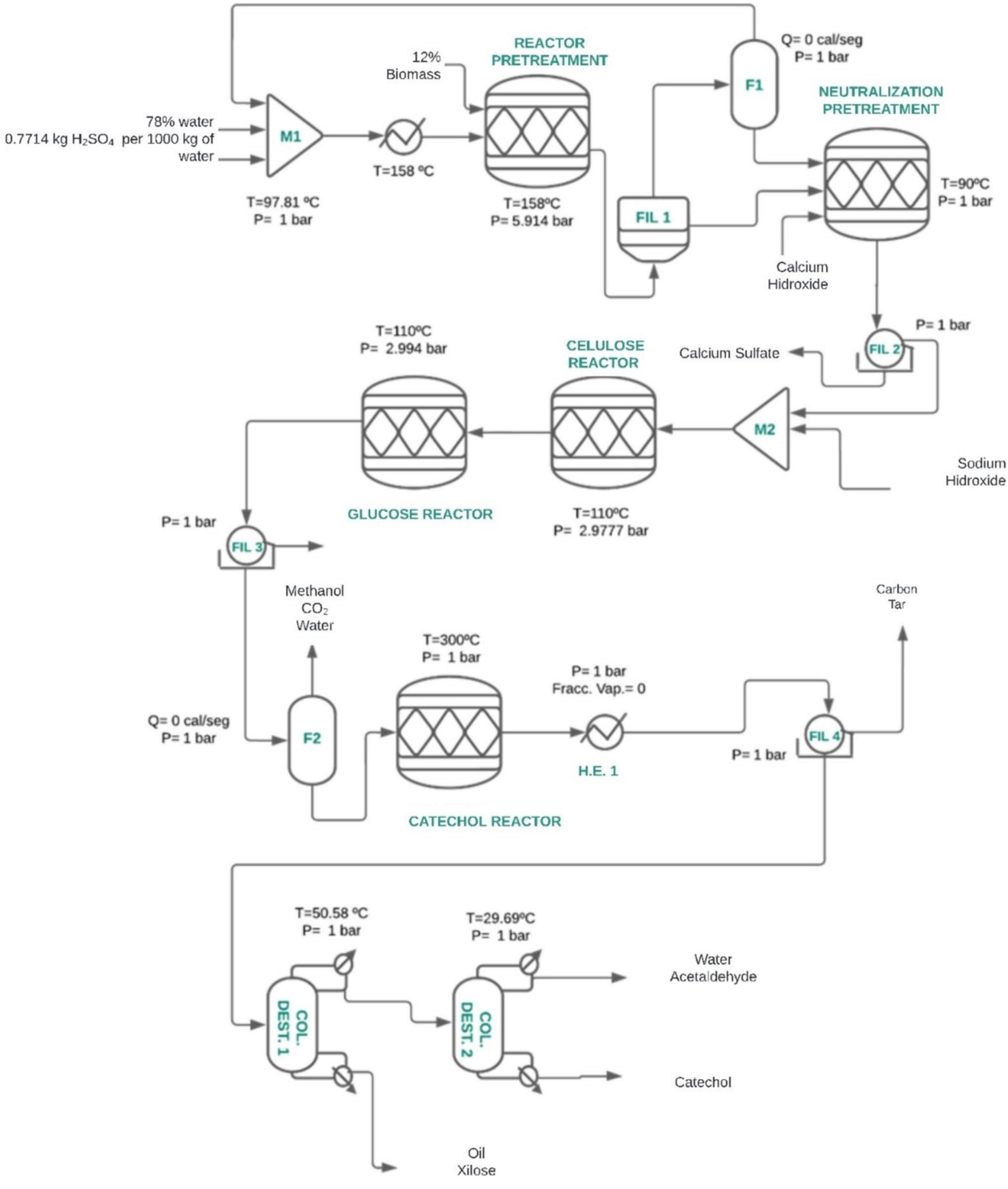


Fig. 1 Dilute acid pretreatment process design

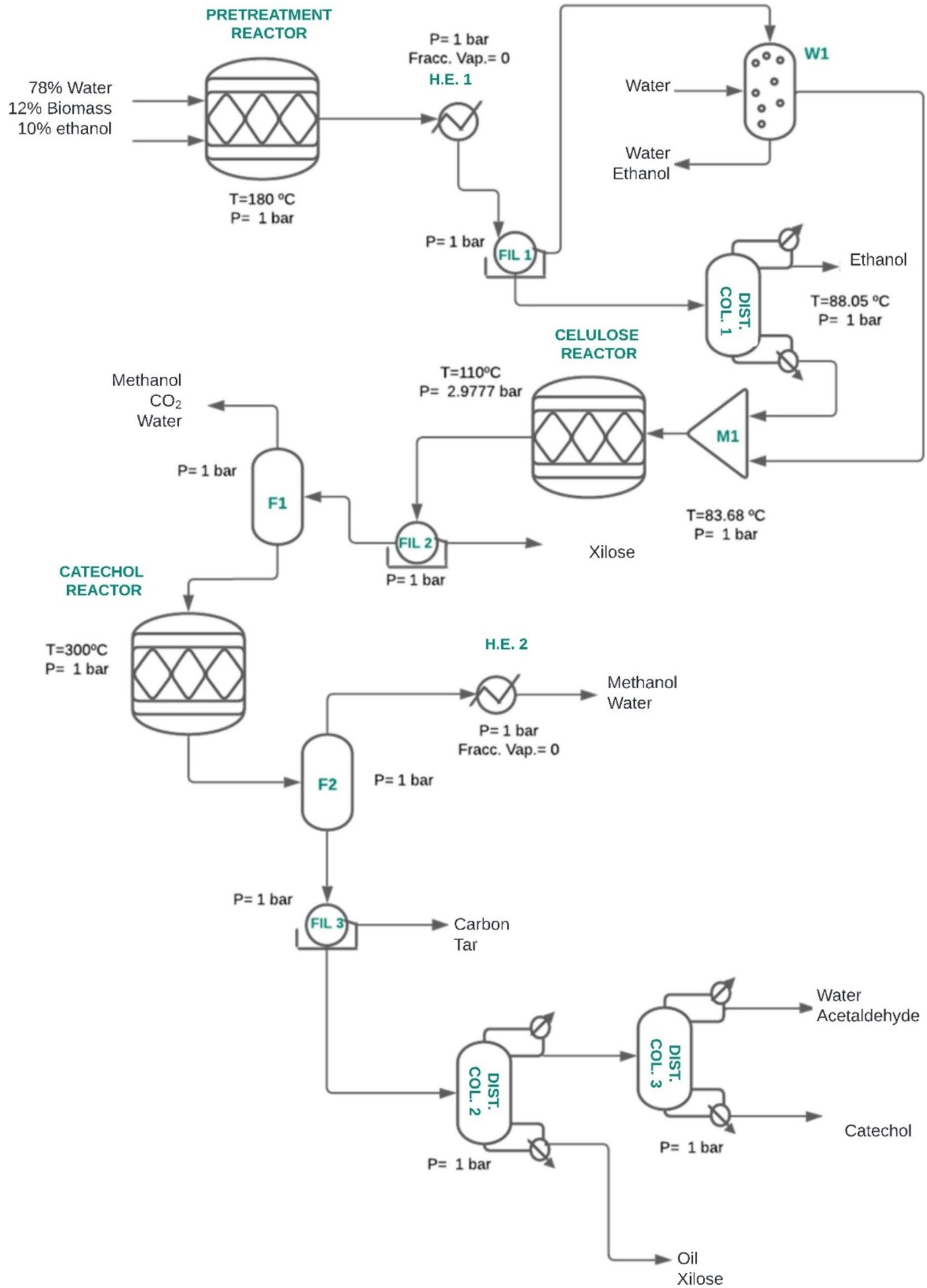


Fig. 2 Organosolv pretreatment process design

Table 1 Average composition (dry basis) for each biomass in mass percent. (Contreras-Zarazúa et al., 2021)

Raw material	Cellulose	Hemicellulose	Lignin
Wheat straw	43.18	29.86	22.37
Corn stover	44.38	26.77	22.37
Sorghum bagasse	44.57	29.25	22.94
Sugarcase bagasse	44.84	25.06	24.43

process. ROI is defined as the net profit (P) divided by the total investment (I).

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

where:

- P is the net profit
- I is the total investment

This indicator clearly shows the financial returns generated from the investment in the production process, highlighting its economic viability and potential profitability. A higher ROI indicates a more profitable process, which is essential for the sustainability and growth of the production facility.

Environmental Indicator: Eco-Indicator 99

The Eco-Indicator 99 (EI99) is a comprehensive environmental assessment tool that evaluates the lifecycle impact of the production process based on three key areas: human health, ecosystem quality, and resource depletion. This indicator aggregates various environmental impacts into a single score, making it easier to compare and minimize overall environmental burdens. Higher EI99 values indicate greater environmental impact.

$$EI99 = \sum_i \omega \bullet C_i \bullet \alpha \tag{2}$$

where:

- ω = weighting factor for damage, reflecting the relative importance of different impacts.
- C_i = impact value for category i, quantifying the effect of specific environmental factors.
- α = quantity being evaluated, representing the amount of substance or energy.

By reducing the EI99 score, the production process can decrease its negative effects on human health, ecosystems, and resource availability.

For the calculation of EI99, impact categories of the compounds and services involved in the process, as well as the steel used in equipment manufacturing, are considered. These factors are measured in points per kWh for electricity and points per kg for services, steel, and substances involved (Table 9).

Safety Indicator: Inherent Safety Index

The Inherent Safety Index (IR) is an essential metric for assessing the safety of the catechol production process. It evaluates the risk based on the frequency of incidents and the probability of their impact. A lower IR indicates a safer process, reducing the likelihood of accidents, health hazards, and environmental damage.

$$IR = \sum_i f_i \bullet P_{x,y} \tag{3}$$

where:

- f_i = frequency of occurrence of incident iii, indicating how often an incident might occur.
- $P_{x,y}$ = probability of impact from incident iii, reflecting the severity of potential consequences.

Table 2 Reactions and conversions in dilute acid pretreatment reactor (Contreras-Zarazúa et al., 2020)

Reaction	Conversion (%)	Equation number
$\mathbf{C_5H_8O_4 + H_2O \rightarrow C_5H_{10}O_5}$	90 (xylan)	(1)
$\mathbf{C_5H_{10}O_5 + H_2O \rightarrow C_6H_{12}O_6}$	9.9 (glucan)	(2)
$\mathbf{C_5H_{10}O_5 \rightarrow C_5H_4O_2 + 3H_2O}$	9 (xylose)	(3)
$\mathbf{2C_5H_{10}O_5 \rightarrow 5C_2H_4O_2}$	8 (xylose)	(4)
$\mathbf{C_5H_{10}O_5 \rightarrow 5CH_4O}$	8 (xylose)	(5)
$\mathbf{C_{10}H_{13.9}O_{1.3} \rightarrow (C_{10}H_{13.9}O_{1.3})_{Sol}}$	5 (lignin)	(6)

Table 3 Reactions and conversions in neutralization reactor (Contreras-Zarazúa et al., 2020)

Reaction	Conversion (%)	Equation number
$\mathbf{Ca(OH)_2 + H_2SO_4 \rightarrow CaSO_4 + 2H_2O}$	100 $Ca(OH)_2$	(7)

Table 4 Reactions and conversions in cellulose reactor (Contreras-Zarazúa et al., 2020)

Reaction	Conversion (%)	Equation number
$\mathbf{C_5H_8O_4 + 3H_2O \rightarrow 4CH_4O + 2CO_2}$	100 (cellulose)	(8)
$\mathbf{C_5H_{10}O_5 + H_2O \rightarrow 2.5C_2H_4O_2}$	100% (hemicellulose)	(9)
$\mathbf{C_{10}H_{13.9}O_{1.3} \rightarrow (C_{10}H_{13.9}O_{1.3})_{Sol}}$	43% (lignin)	(10)

Table 5 Reactions and conversions in glucose reactor (Contreras-Zarazúa et al., 2020)

Reaction	Conversion (%)	Equation number
$C_6H_{12}O_6 + 2H_2O \rightarrow 4CH_4O + 2CO_2$	100% (glucose)	(11)
$1.5C_5H_8O_4 + 1.5H_2O \rightarrow 3.75C_2H_4O_2$	100% (hemicellulose)	(12)

Table 6 Reactions and conversions in catechol reactor (Mabrouk et al. 2018)

Reaction	Conversion (%)	Equation number
$(Lignin)_{Sol} \rightarrow 0.075OleicAcid + 0.026Catechol + 0.004Tar + 0.789CH_3OH + 0.33H_2O + 0.908C$	100 $(Lignin)_{Sol}$	(13)

Minimizing the IR is crucial for ensuring a safe working environment, protecting employees, and maintaining regulatory compliance.

In the assessment of the IR, the analysis includes specific incidents relevant to the catechol production process, such as (Medina-Herrera et al. 2014):

Gas pipeline leaks with a probability derived from the frequency of pipeline material failures.

Liquid pipeline leaks, considering scenarios with partial and full rupture probabilities, based on historical data and risk models.

Catastrophic equipment failures, such as explosions and fires, using failure rates and consequence probabilities.

Continuous and instantaneous hazardous substance releases, where dispersion and impact probabilities were calculated using fault and event trees, aligned with quantitative risk analysis (QRA) standards.

Table 7 Reactions and conversions in organosolv pretreatment reactor (Mabrouk et al. 2018)

Reaction	Conversion (%)	Equation number
$C_5H_8O_4 + H_2O \rightarrow C_5H_{10}O_5$	32.2 (cellulose)	(14)
$C_5H_{10}O_5 + H_2O \rightarrow C_6H_{12}O_6$	1.984 (hemicellulose)	(15)
$C_{10}H_{13.9}O_{1.3} \rightarrow (C_{10}H_{13.9}O_{1.3})_{Sol}$	68.1 (lignin)	(16)

Process Optimization

Process optimization was performed using the DETL algorithm, combining differential evolution and tabu search techniques. The algorithm involves the following steps (Srinivas & Rangaiah 2007):

Generation: Randomly generate vectors within a limited range for each generation, representing possible solutions.

Table 8 Reactions and conversions in catechol reactor (Mabrouk et al. 2018)

Reaction	Conversion (%)	Equation number
$(Lignin)_{Sol} \rightarrow 0.075OleicAcid + 0.026Catechol + 0.004Tar + 0.789CH_3OH + 0.33H_2O + 0.908C$	100 $(Lignin)_{Sol}$	(18)

Table 9 Weighting factors for impact categories (Quiroz-Ramírez et al. 2017)

Impact category	Electricity (pts/kWh)	Steam (pts/kg)	Steel (pts/kg)	Water (pts/kg)
Carcinogens	1.29×10^{-3}	1.04×10^{-4}	6.32×10^{-3}	2.87×10^{-6}
Organic compounds	1.01×10^{-5}	1.56×10^{-3}	8.01×10^{-2}	1.32×10^{-5}
Climate change	4.07×10^{-3}	1.27×10^{-3}	1.31×10^{-2}	4.35×10^{-6}
Radiation	8.94×10^{-5}	1.91×10^{-6}	4.51×10^{-4}	4.17×10^{-7}
Ozone layer	5.41×10^{-7}	7.78×10^{-7}	4.55×10^{-6}	1.63×10^{-8}
Ecotoxicity	2.14×10^{-4}	2.85×10^{-4}	7.45×10^{-2}	1.80×10^{-6}
Acidification/eutrophication	9.88×10^{-4}	1.21×10^{-4}	2.71×10^{-3}	9.52×10^{-7}
Land use	4.64×10^{-4}	8.60×10^{-5}	3.73×10^{-3}	1.70×10^{-6}
Minerals	5.85×10^{-5}	8.87×10^{-6}	7.42×10^{-2}	1.27×10^{-6}
Fossil fuels	1.010E-02	1.240E-02	0.059	1.550E-05

Mutation: Create a perturbation from a parent vector to generate a donor vector, which is then recombined with the target vector.
Crossover: Exchange components between the mutant and target vectors to form a trial vector, controlled by a probability factor (C_r).
Selection: Evaluate individuals to maintain constant population size, determining if the target or trial vector survives to the next generation.

The algorithm iterates until a global solution is found or a maximum number of generations is reached. Tabu List parameters include Tabu Radius and Tabu List Size, preventing reevaluation of previously assessed points.

For the implementation of the DETL method, a hybrid platform is necessary, which involves linking Microsoft Excel, the Aspen Plus process simulator, and Visual Basic. The optimization algorithm is programmed in Excel through a Visual Basic macro as follows:

a. To start the optimization process, the design variables are specified in Microsoft Excel. Using the DETL algorithm programmed in Excel through a Visual Basic macro, initial values are randomly selected. These initial values are then passed to Aspen Plus, where they are used as input data to simulate the proposed design. Mass and energy balances are also resolved in this step.
b. The results obtained are sent back to Excel, where the data are stored.

Finally, with all the resulting data, the objective function values are analyzed, and new values for the decision variables are proposed according to the DETL algorithm looking to get a 98% of catechol's purity. The parameters used for the optimization process were: 200 individuals, 1000 maximum number of generations, a taboo list of 50% of total individuals, a taboo radius of $1 \times 10-6$, 0.8 and 0.6 for crossover probability and mutation factor, respectively. These parameters were obtained from the literature and tuning process via preliminary calculations (Srinivas and Rangaiah 2007).

This multi-objective minimization considered 25 continuous and discrete variables. Note that the product streams flows are manipulated and the recoveries of the key components in each product stream must be included as a constraint for the optimization problem. Tables 10 and 11 show the decision variables for the dilute acid and organosolv processes, respectively.

Table 10 Decision variables for dilute acid process

Decision variable	Range	Units
Column acetaldehyde: number of stages	3–90	-
Column acetaldehyde: feed stage	3–89	-
Column acetaldehyde: reflux ratio	1–13	-
Column acetaldehyde: distillate flow	20–92	kg/h
Column acetaldehyde: diameter	0.5–3	m
Column catechol: number of stages	3–40	-
Column catechol: feed stage	3–39	-
Column catechol: reflux ratio	1–13	-
Column catechol: distillate flow	20–90	kg/h
Column catechol: diameter	0.5–3.5	m

Table 11 Decision variables for organosolv process

Decision variable	Range	Units
Column ethanol: number of stages	3–100	-
Column ethanol: feed stage	3–99	-
Column ethanol: reflux ratio	1–13	-
Column ethanol: bottom flow	3000–7000	kg/h
Column ethanol: diameter	0.5–2	M
Column acetaldehyde: number of stages	3–50	-
Column acetaldehyde: feed stage	3–49	-
Column acetaldehyde: reflux ratio	1–16	-
Column acetaldehyde: distillate flow	100–1000	kg/h
Column acetaldehyde: diameter	0.5–3	m
Column catechol: number of stages	3–55	-
Column catechol: feed stage	3–54	-
Column catechol: reflux ratio	1–16	-
Column catechol: distillate flow	20–90	kg/h
Column catechol: diameter	0.5–3.5	m

Objective Function

The objective function integrates the economic, environmental, and safety indicators to optimize the catechol production process. The aim is to find the best balance between maximizing ROI and minimizing EI99 and IR.

$$min[EI99, IR, -ROI] = f(x, y, z) \quad (4)$$

where x, y, z represent the decision variables that influence the process. The purpose is to determine the optimal values for these variables that achieve the desired outcomes.

Equation 4 considers equal weightage for the three indicators: EI99, IR, and ROI. This approach ensures that all objectives are treated with the same level of importance during the optimization process, reflecting a balanced evaluation of environmental impact, safety, and economic performance. Assigning equal weights avoids introducing subjective bias into the optimization and allows for a fair trade-off among the objectives.

Assigning equal weightage in Eq. 4 ensures that each of the three objectives—environmental impact (EI99), inherent safety (IR), and economic feasibility (ROI)—is treated with the same importance during the optimization process, thereby avoiding subjective bias from arbitrarily assigned weights. This approach allows for a balanced analysis of trade-offs among objectives, aligned with the study's goals. However, we recognize that this method may not fully capture specific stakeholder priorities or regulatory requirements that could favor certain objectives. To address this, alternative multi-objective optimization approaches have been considered, such as Pareto fronts to identify non-dominated solutions highlighting trade-offs between objectives; weighted sum methods that allow adjusting the emphasis on each objective based on context; normalization techniques to ensure comparability across indicators of different magnitudes; and evolutionary algorithms like NSGA-II, which generate diverse and robust solutions in the decision space. Integrating these approaches complements the analysis and supports the robustness of the proposed optimization framework, ensuring a fair balance among environmental impact, safety, and economic performance.

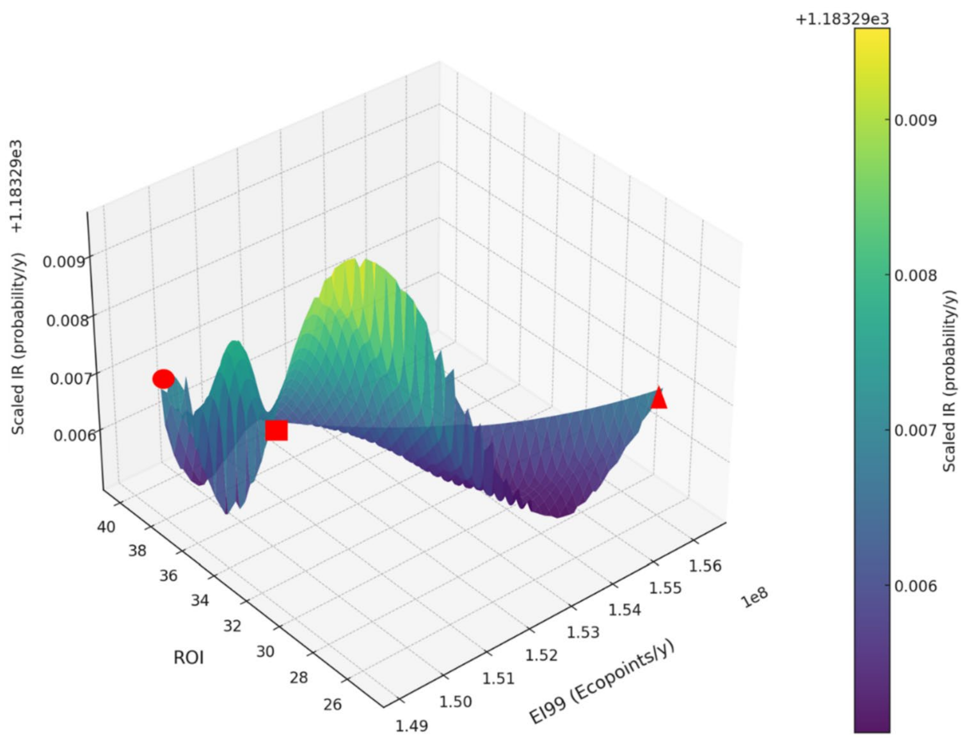
Results and Discussion

The following section will present the results obtained during the modeling and optimization process. As mentioned in the methodology section, two types of pretreatment were considered, dilute acid and organosolv. In that sense, first, the results of the dilute acid and organosolv arrangement are presented.

Subsequently, an analysis will be made of the results obtained from the optimization for the objective functions: cost, control, and EI99 in terms of the process variables. Also, some tables showing the optimal conditions found will be shown in order to analyze and discuss the advantages of the process. All the results shown in the Pareto fronts represent process schemes that satisfy the catechol purity constraint of 98%. This purity constraint is respected by the two pretreatment scenarios considered in this work. In the same sense, the Pareto front represents a set of solutions with some trade-off between the objectives evaluated in the optimization process. Figure 3a–c shows the Pareto front obtained by considering dilute acid as pretreatment from different perspectives.

According to the objective function, the aim is to maximize the ROI, minimize the environmental impact (EI99), and minimize the IR. With this in mind, various tendencies are observed, due to the fact that the zone where the maximums and minimums of the objective functions coexist is sought. Note that there is a compromise between the objective functions due to the characteristics that the model of each function presents. For example, the ROI when

Fig. 3 Optimization results considering dilute acid as pretreatment



On the Pareto front, it is possible to highlight three process alternatives:

A: ▲ Represents the design with lower ROI, higher IR, and higher EI99.
B: ■ Represents the design with medium ROI, lower IR, and medium EI99.
C: ● Represents the design where it has higher ROI, medium IR, and lower EI99.

considering the investment, as well as the profit of the process. In the case of investment, the costs of equipment and services must be considered, so an attempt will be made to minimize both costs. However, the variables that precede both calculations have an opposite tendency.

Thus, the impact of the cost associated with equipment will benefit from equipment with small dimensions (small diameter, columns with few stages); on the other hand, a column with few stages will favor a high reflux ratio/high reboiler duty to achieve the separation that is not achieved with physical equilibrium stages. Small equipment and low capital cost will commonly be associated with high service costs and vice versa.

This same example can be taken to the level of economic impact. EI99 considers the environmental burden associated with the use of energy and steel. In this sense, considering the relationship between variables explained previously, it shows that a process with a low impact on steel use will have a high impact due to energy use.

On the other hand, Fig. 3 also shows the relationship between the safety index (IR) and the other objective functions, highlighting the compromises required to balance them. The safety index is influenced by the amount of mass contained in the equipment, the physicochemical properties of the materials, and the operating conditions. For example, in the case of a distillation column, high reflux ratios lead to increased mass inside the column, as well as higher reboiler duties, pressures, and temperatures. These factors result in a higher safety index, reflecting increased risk. Conversely, operating at lower reflux ratios reduces these risks but requires larger column dimensions, which increase capital costs and the associated environmental impact (EI99). This trade-off illustrates how changes in process variables affect safety, economic, and environmental metrics, emphasizing the importance of balancing these objectives to achieve an optimal design. This relationship is particularly evident in the Pareto front, where designs such as A exhibit lower ROI, higher safety index, and higher EI99 due to the energy and material requirements.

Then, again, the safety index, which is evaluated jointly with the other objective functions, through the optimization process should find the best operating conditions to achieve the best compromise between the functions. Figure 3c shows the relationship between the Safety Index and the Return on Investment, showing an antagonistic behavior. To obtain a safer process the economic investment will be larger.

This tendency is linked to the reboiler duty and dimensions of the equipment (volume), if there are higher reboiler duty there will be an increase in operating costs and heating services and therefore a direct decrease in the ROI. A similar behavior happens with the equipment, the larger the volume, the higher the cost for its manufacture will increase, and therefore the ROI will be lower.

According to the data shown in the Pareto front, Table 12 shows the design data of the three process alternatives present in Fig. 3.

Table 12 indicates that configuration A, with the highest reboiler duty (4.776×10^5 cal/s), also has the highest catechol production (11.065 kg/h) but results in the highest EI99 (4,163,722.18 pts/kg catechol) and the lowest ROI (28.577%) due to its elevated energy consumption. In contrast, configuration C achieves the lowest EI99 (4,067,888.28 pts/kg catechol) and the highest ROI (33.511%) by optimizing reboiler duties and energy requirements, despite its slightly larger equipment size. Regarding the Inherent Safety Index (IR), configuration A exhibits a marginally higher value (0.00145967) due to increased hazardous material inventory associated with high reflux ratios and reboiler duties. Configuration B achieves the lowest IR (0.00145959) by maintaining a balance between reduced inventory and efficient operating conditions. These findings underscore the trade-offs between energy efficiency,

Table 12 Design parameter of diluted acid alternatives

Design parameters	A	B	C
Column 1			
Stages	54	55	56
Feed stage	53	54	55
Reflux ratio	72.12	67.53	64.38
Distillate flow (kg/h)	73.95	73.39	73.47
Diameter (m)	2.096	2.447	1.59
Height (m)	31.69	32.30	32.91
Reboiler duty (cal/s)	4.776×10^5	4.479×10^5	4.303×10^5
Column 2			
Stages	30	27	26
Feed stage	27	3	5
Reflux ratio	63.62	42.88	41.35
Distillate flow (kg/h)	62.67	62.77	62.79
Diameter (m)	1.58	1.61	1.259
Heigh (m)	17.06	15.24	14.63
Reboiler duty (cal/s)	2.862×10^5	1.948×10^5	1.88×10^5
Flash			
Temperature (ºC)	123.27	123.19	123.18
Indices			
Catechol production (kg/h)	11.06	10.40	10.97
EI 99 (pts/kg catechol)	4,163,722	4,088,039	4,067,888
IR	0.00145967	0.00145959	0.0014596
ROI (%)	28.577	33.205	33.511

environmental impact, and safety in the dilute acid process and highlight the importance of optimizing process parameters to achieve a balanced design.

It can also be observed that the configuration with the best ROI is C (33.51%) and the lowest EI99 (4,067,888.28 pts/kg catechol), this can be explained by the values of the reboiler duty, which are the lowest of the 3 configurations presented.

Regarding the process scheme that considers organosolv as pretreatment. The Pareto front in Fig. 4 shows the behavior observed in the optimization process.

In general, similar trends to those observed in Fig. 4, but shifted to different values. These trends, mostly antagonistic, are influenced by the size of the equipment and reboiler duty. With larger equipment sizes, the amount of steel required will be greater. In this case, distillation columns with a larger number of plates or diameters will require more energy expenditure, directly increasing the EI99.

Some trends in terms of safety associated with the process have been mentioned. Additionally, it is possible to infer some behavior in terms of other types of properties. For example, having larger equipment will have an impact on the calculation of the safety index. It can also be inferred that a larger equipment will have less impact on the controllability of the process as mentioned with some authors (Sánchez-Ramírez et al. 2022).

According to the Pareto observed in Fig. 4, it is possible to highlight three alternatives as good solutions. The design parameters of these equipment can be seen in Table 13.

Table 13 shows that the highest amount of catechol (43.1 kg/h) is obtained at the point with columns with the highest reflux ratio and reboiler duties, having a high EI99

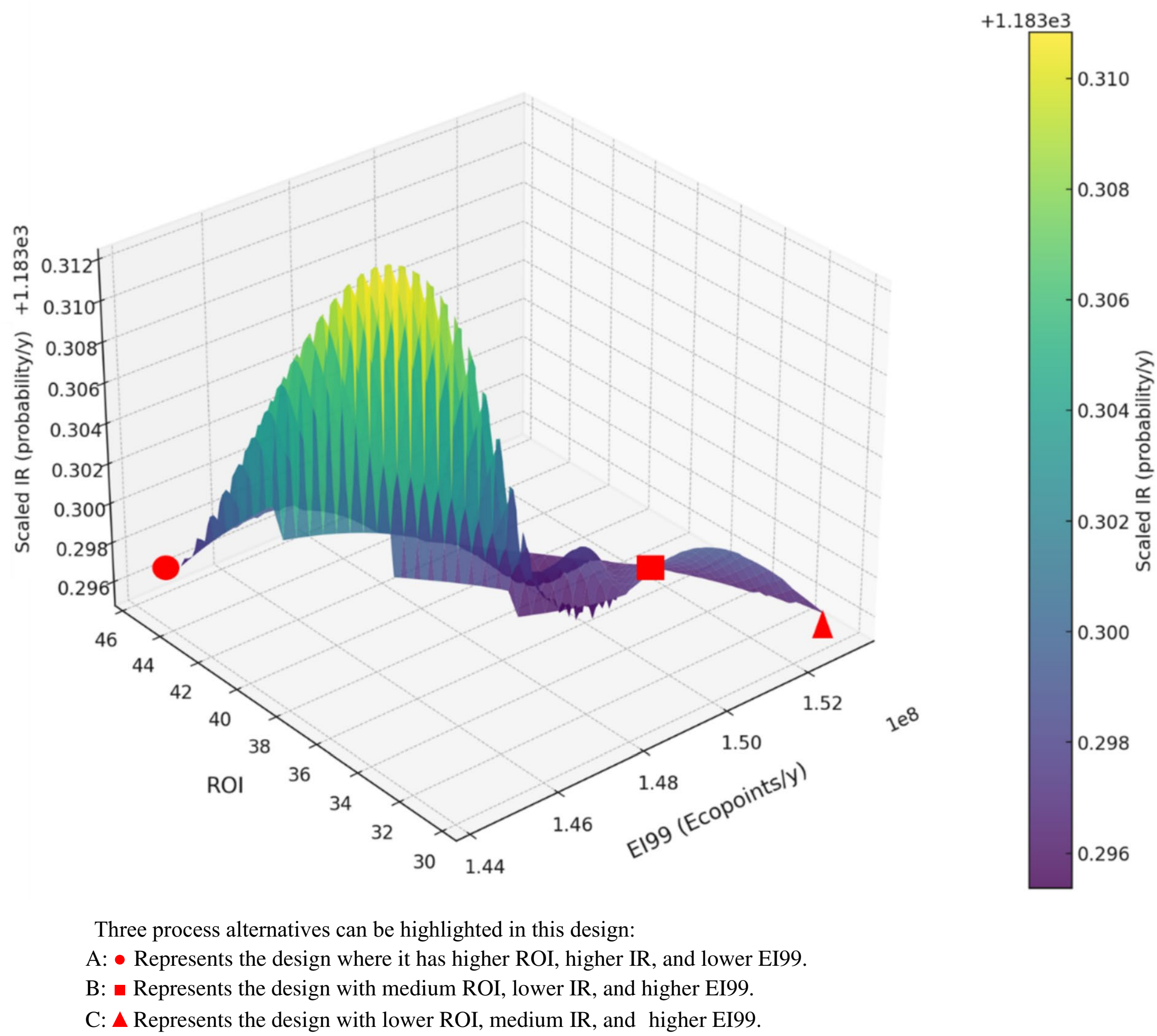


Fig. 4 Optimization results considering organosolv as pretreatment

Table 13 Design parameter of organosolv alternatives

Design parameters	A	B	C
Column 1			
Stages	79	79	79
Feed stage	78	78	78
Reflux ratio	88.01	87.656	87.54
Distillate flow (kg/h)	77.05	77.12	77.09
Diameter (m)	2.20	2.25	2.28
Height (m)	46.93	46.93	46.93
Reboiler duty (cal/s)	1,568,474	1,568,474	1,568,474
Column 2			
Stages	83	83	83
Feed stage	44	45	44
Reflux ratio	54.15	54.23	54.18
Distillate flow (kg/h)	33.54	33.48	33.43
Diameter (m)	1.54	1.54	1.54
Height (m)	49.37	49.37	49.37
Reboiler duty (cal/s)	1.15×10^5	1.131×10^5	1.155×10^5
Column 3			
Stages	69	71	69
Feed stage	42	49	43
Reflux ratio	117.62	127.37	126.27
Distillate flow (kg/h)	7466.29	7369.74	7389.04
Diameter (m)	3.06	0.89	2.55
Height (m)	40.84	42.06	40.84
Reboiler duty (cal/s)	1.121×10^8	1.195×10^8	1.188×10^8
Flash 1			
Temperature (ºC)	146	145	145
Flash 2			
Pressure (atm)	12.20	12.24	12.13
Indices			
Catechol production (kg/h)	42.84	42.73	43.10
EI 99 (pts/kg catechol)	$1.05\text{E}\times10^8$	1.11×10^8	1.11×10^8
IR	0.0014282185	0.00142821294	0.0014282142529
ROI (%)	41.4	30.7	30.4

(1.11×10^8 pts/kg catechol), the lowest ROI (30.427%) and the highest IR (0.0014282142529).

In Table 13, the EI99 score is primarily influenced by energy use (reboiler duties) and material consumption (equipment size). Configuration A achieves the lowest EI99 (1.05×10^8 pts/kg catechol) and the best ROI (41.46%) due to its lower energy requirements, as reflected in its reduced reboiler duty values. In contrast, configurations B and C, with larger heigh and higher reboiler duties, show higher EI99 scores (1.11×10^8 pts/kg catechol) and lower ROI values (30.7% and 30.4%, respectively), highlighting the environmental and economic penalties of increased energy consumption.

Similarly, the Inherent Safety Index (IR) is affected by hazardous material inventory and operating conditions. Configuration B achieves a slightly lower IR (0.00142821294) by reducing the inventory and optimizing conditions, while configuration A shows the highest IR (0.0014282142529) due to its higher reflux ratio and reboiler duty. These results emphasize the trade-offs between safety, environmental impact, and economic feasibility, demonstrating the importance of balancing these objectives to achieve optimal process performance.

The trade-offs between ROI, EI99, and IR are evident across both pretreatments and their respective configurations, reflecting the multifaceted challenges of process optimization. For dilute acid pretreatment, achieving higher catechol production often entails elevated energy consumption and larger equipment sizes, directly influencing both EI99 and IR. While configuration C minimizes these impacts through improved energy efficiency, configuration A demonstrates that prioritizing production rates can significantly compromise environmental and safety metrics.

In contrast, the organosolv pretreatment shows a distinct pattern where its inherently higher efficiency in lignin solubilization translates to a better ROI across configurations. However, this advantage is offset by the environmental penalties of increased material flows and energy demands, as seen in the higher EI99 scores. Despite this, configuration A in organosolv achieves a unique balance by leveraging reduced reboiler duties to maintain a lower EI99 while also achieving competitive catechol production levels.

When comparing the pretreatments, the trade-offs emphasize that dilute acid offers a pathway to moderate impacts across all objectives, favoring balanced designs. Conversely, organosolv is more suitable for maximizing economic returns but requires mitigation strategies to address its higher environmental burden. This comparison underscores the importance of aligning process design with specific operational priorities, whether they emphasize economic feasibility, environmental responsibility, or inherent safety.

In this study, the Return on Investment (ROI) was evaluated as the primary economic metric for assessing the catechol production plant. However, an additional analysis was conducted considering an exponential growth model for the production capacity of the plant. Such scenarios are particularly useful for understanding the initial economic performance and production potential of a new facility. This type of analysis provides valuable insights into how production capacity evolves over time, especially during the ramp-up phase, and its impact on economic outcomes. Similar methodologies have been preliminarily presented to evaluate various case studies (Mendoza-Ortega et al. 2021; Surbier et al. 2014), which explores scenario-based modeling for aggregate production planning in a production company. The complete calculation, which projects the production scenario using this methodology, is provided in full detail in the Supplementary Material. This approach serves as a foundational tool for strategic decision-making in the early stages of plant operation and expansion.

Conclusions

This work presents a simultaneous optimization for catechol production from corn stover using the Differential Evolution with Tabu List (DETL) stochastic optimization methodology. The objective was to find the optimal design by reducing environmental impacts and maximizing the Return On Investment. The optimization results indicate the potential to achieve multiple designs with a catechol purity of 98%, enhanced recovery, maximized Return On Investment, and minimized safety index and eco-points. In the case of Dilute Acid treatment, optimal conditions, such as reflux ratios of 72.12 and 63.62, and distillate flows of 73.95 and 62.67 kg/h for columns 1 and 2, respectively, were crucial for achieving higher purity catechol. For the Organosolv treatment, optimal conditions included reflux ratios of 88.0097, 54.1539, and 117.6262, and distillate flows of 77.05, 33.54, and 7466 kg/h for columns 1, 2, and 3, respectively.

The choice of pretreatment significantly affects lignin yield upon separation and solubilization. When comparing the two pretreatments, Organosolv produced approximately 390% more catechol flow than dilute acid. However, organosolv exhibited a higher environmental impact (1.11×10^8 pts/kg catechol versus 4.07×10^6 pts/kg catechol for dilute acid), but also achieved a better Return On Investment (41% compared to 33%) and a slightly lower safety index (0.0014282 versus 0.0014596).

From a sustainability standpoint, this study successfully identified two designs for catechol production that balance environmental impact, economic viability, and safety. These designs support the concept of a complete biorefinery, utilizing cellulose, hemicellulose, and lignin to maximize the production of high-value products. Importantly, these designs increase lignin utilization beyond the current 2% used for high-value chemicals, thereby addressing lignin underutilization. This research demonstrates the feasibility of applying advanced optimization methodologies to develop sustainable and economically viable processes for catechol production from lignin-rich biomass. It highlights how agricultural waste can be transformed into valuable products, advancing greener and more efficient industrial practices and setting a precedent for future biorefinery innovations. Moreover, in this work, a preliminary calculation was presented to project the production scenario over a 5-year period. This calculation, while simple and preliminary, provides valuable insights for the economic evaluation and production growth of a new plant. Such an analysis is particularly useful for gaining an initial understanding of how production capacity and economic performance evolve over time during the ramp-up phase, providing a foundational tool for strategic planning and future decision-making in biorefinery development. Furthermore, this work shows the potential for establishing a biorefinery based on lignin, supported by the idea that integrating processes can enhance overall efficiency and yield of valuable products. This indicates that with advancements in reaction engineering and catalyst design, it is feasible to develop processes that can industrially convert lignin into a range of high-value-added compounds, thereby contributing to a more sustainable and circular economy.

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Data Availability Data is available on request from the authors.

Declarations

Conflict of interest The authors declare no competing interests.

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