



A multi-approach assessment of a low-TRL lignocellulosic biorefinery for lignin production

Rafic El Kazzi, Carlos Eduardo Robles-Rodriguez, Ligia Tiruta-Barna^{*}, Aras Ahmadi

TBI, Université de Toulouse, CNRS, INRAE, INSA, Toulouse, France

ARTICLE INFO

Keywords:

Low-TRL Life Cycle Assessment
Process eco-design and simulation
Scaled-up foreground modeling
Parametric analysis
Dynamic LCA
Prospective LCA

ABSTRACT

Lignocellulosic biorefineries have gained interest as sustainable bio-based alternatives to replace fossil-based technologies. However, the processes to treat lignocellulose are still at low Technology Readiness Levels (TRL), which difficult comparison with their well-established high-TRL fossil counterparts. This study proposes a comprehensive multi-approach assessment of technical and environmental performances of a low-TRL organo-solv process applied to lignin production from lignocellulosic biomass. A simulation-based approach was implemented to scale-up patent data for the American Science and Technology (AST) process, and compared with a simplified method based on chemical engineering laws. The resulting input/output flows for each process step were automatically coupled with LCA tools (Brightway2, Activity Browser, ecoinvent 3.9.1) for environmental impact calculation (with Environmental Footprint 3.1 method). Life Cycle Assessment (LCA) disclosed a tradeoff between solvent recovery and energy consumption, determining the competitiveness of AST regarding the climate change impact (1.2 kg CO₂-eq). Pearson, sensitivity, principal component and uncertainty analyses were conducted on 20 process parameters, 9 performance and 24 impact indicators. Biomass composition, lignin dissolution conversion, cake moisture in filtration steps, and distillate flowrate showed as the most sensitive parameters for the most representative process performance indicators: lignin yield, water consumption, total heat demand, and GWP₁₀₀. Dynamic LCA demonstrated a temporal climate benefit of lignin produced by AST and used in materials, which disagrees the static LCA result. Prospective LCA (Premise tool, for 2020–2050) highlighted a slight decrease in climate change correlated with the increase in mineral/metal resource depletion, due to the electricity defossilization and increased nuclear and renewable power contributions.

List of acronyms

AST	American Science and Technology
AST-HC	Scenario AST with simplified calculation of inventory
AST-SR	Scenario AST with enhanced solvent recovery
dLCA	Dynamic Life Cycle Assessment
EF	Environmental Footprint
Fr	France
FU	Functional unit
GHG	Greenhouse Gas
GMTC	Global mean temperature change
IAM	Integrated Assessment Model
IMAGE	Integrated Model to Assess the Global Environment
iRF	Cumulated radiative forcing
ISO	International Organization for Standardization

LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life Cycle Impact Assessment
MW	Molecular weight
OAT	One at a time
PCA	Principal Component Analysis
pLCA	Prospective Life Cycle Assessment
PFD	Process Flow Diagram
RER	Europe
REMIND	Regional Energy Model with Induced Detail
RFI	Request for Information
RoW	Rest of World
SI	Supplementary Information
SSP2-NDC	Shared Socioeconomic Pathway 2 – Nationally Determined Contributions

^{*} Corresponding author.

E-mail addresses: el-kazzi@insa-toulouse.fr (R. El Kazzi), roblesro@insa-toulouse.fr (C.E. Robles-Rodriguez), lbarna@insa-toulouse.fr (L. Tiruta-Barna), ahmadi@insa-toulouse.fr (A. Ahmadi).

<https://doi.org/10.1016/j.biteb.2026.102829>

Received 24 February 2026; Received in revised form 25 April 2026; Accepted 19 May 2026

Available online 21 May 2026

2589-014X/© 2026 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

TRL Technology Readiness Level

Impact Assessments of the Method Environmental Footprint (EF v3.1)

ADP	Material resources: metals/minerals, abiotic depletion potential: elements (ultimate reserves)
AE	Acidification, accumulated exceedance
AE (terrestrial)	Eutrophication: terrestrial, accumulated exceedance
CTUe	Ecotoxicity: freshwater, comparative toxic unit for ecosystems
CTUe (Inorganic)	Ecotoxicity: freshwater, inorganics, comparative toxic unit for ecosystems
CTUe (organic)	Ecotoxicity: freshwater, organics, comparative toxic unit for ecosystems
CTUh (C)	Human toxicity: carcinogenic, comparative toxic unit for human
CTUh (Inorganics)	Human toxicity: carcinogenic, inorganics, comparative toxic unit for human
CTUh (Organics)	Human toxicity: carcinogenic, organics, comparative toxic unit for human
CTUh (N.C)	Human toxicity: non-carcinogenic, comparative toxic unit for human
CTUh (N.C: Inorganics)	Human toxicity: non-carcinogenic, inorganics, comparative toxic unit for human
CTUh (N.C: Organics)	Human toxicity: non-carcinogenic, organics, comparative toxic unit for human
fossil fuels	Energy resources: non-renewable, abiotic depletion potential: fossil fuels
GWP ₁₀₀	Climate change, global warming potential
GWP ₁₀₀ (biogenic)	Climate change: biogenic, global warming potential
GWP ₁₀₀ (fossil)	Climate change: fossil, global warming potential
GWP ₁₀₀ (L.U.C)	Climate change: land use and land use change, global warming potential
Land use	Land use, soil quality index
N (marine)	Eutrophication: marine, fraction of nutrients reaching marine end compartment
ODP (Ozone)	Ozone depletion, ozone depletion potential
P (Freshwater)	Eutrophication: freshwater, fraction of nutrients reaching freshwater end compartment
PM25	Particulate matter formation, impact on human health
PO	Photochemical oxidant formation: human health, tropospheric ozone concentration increase
u235	Ionising radiation: human health, human exposure efficiency relative to u235
Water use	Water use, user deprivation potential (deprivation-weighted water consumption)

1. Introduction

As the transition toward a bio-based economy accelerates, emerging technologies for converting biomass into valuable materials are gaining increasing attention. However, most innovations remain at low Technology Readiness Levels (TRLs), making difficult to evaluate their technical feasibility and environmental sustainability. Laboratory data are often specific to experimental conditions and cannot be directly extrapolated to industrial scales (Simon et al., 2016). This lack of robust information hampers decision-making for research prioritization and policy development. Life Cycle Assessment (LCA) is a standardized methodology, defined by ISO 14040 (ISO, 2006a) and 14044 (ISO, 2006b), used to evaluate the environmental impacts of a product throughout its life cycle. It enables the assessment of new technologies and their comparison with established, high-TRL processes. Such comparisons require scaling up the inventory data of low-TRL systems to represent full-scale implementation (Romina et al., 2025).

The extraction of lignin from lignocellulosic biomass represents a promising pathway for the development of integrated biorefineries. Lignocellulosic feedstocks are globally abundant and composed of three

major fractions: cellulose, hemicellulose, and lignin (Segers et al., 2024). Traditionally, lignin extraction at both industrial and laboratory scales has relied on acid sulfite and kraft pulping processes (Zeilerbauer et al., 2021). Other fractionation processes have been developed. For example, thermochemical approaches such as steam explosion rely on autohydrolysis under high temperature and pressure, but often lead to lignin condensation and reduced valorization potential (Alvira et al., 2010). Alkaline-based processes such as Kraft pulping are industrially mature and highly effective for delignification; however, they require intensive chemical recovery systems and generate chemically modified lignin streams (Watkins and Fatehi, 2026). Acid-catalyzed fractionation routes provide efficient carbohydrate hydrolysis but suffer from equipment corrosion and the formation of inhibitory degradation products (Li et al., 2018). In parallel, emerging solvent-based systems such as deep eutectic solvents (DES) have demonstrated the ability to preserve lignin structure, enabling higher-value applications; however, their industrial deployment remains constrained by issues related to solvent cost, stability, and recovery (Alsoy Altinkaya, 2024). Finally, organosolv processes represent a compromise between performance and scalability, offering relatively high lignin purity and process flexibility while still facing challenges related to solvent recovery and energy demand (Zeilerbauer et al., 2021). Organosolv process produces high-purity, sulfur-free lignin with minimal impurities, improving its suitability for high-value applications (Zhao et al., 2009). Preservation of β -O-4 linkages during organosolv treatment increases the chemical reactivity of lignin, facilitating downstream functionalization (Lange et al., 2013). The process also offers flexibility across biomass types, from hardwoods to agricultural residues, broadening its industrial potential (Reith et al., 2008).

Various organosolv systems have been explored, including Alcell and Acetosolv, while newer processes such as Bloom and the Fraction project are under development (Tofani et al., 2023). Typical solvents include ethanol and acetic acid, often combined with sulfuric acid as a catalyst. Among these, the organosolv process developed by American Science and Technology (AST) stands out for its use of butanol as the main solvent and sulfuric acid as catalyst, enabling high lignin purity, although currently at a low TRL, but with strong potential for industrial scale-up (Manesh et al., 2014). The main barriers to scaling up organosolv processes remain their high energy demand and solvent recovery, which can be mitigated through optimized unit operations, energy efficiency, and renewable low-carbon sourcing (Herry, 2020).

LCA studies on lignin have grown significantly over the past decade, from an initial 62 peer-reviewed articles, 48 studies specifically addressed the LCA of lignin or lignin-derived products, with 42 published within the last ten years and approximately 85% appearing in the past five years (Scopus preview, 2026). The 41 laboratory-scale studies can be categorized by product system: Kraft lignin (3 studies), organosolv lignin (1), biorefinery delignification using natural malic acid (1), lignin-based applications (15), major biorefinery products such as ethanol (21), and meta-analyses of bio-based chemicals including lignin-derived products (1) (Moretti et al., 2021). Most biorefinery-focused LCAs targeted low-TRL processes, more than half relied partially on primary data generated at the laboratory scale, which were then scaled-up to approximate large-scale performance. About 28% used fully modeled data from simulation tools without experimental validation, while roughly 18% relied only on secondary literature or LCA database data. This distribution highlights the limited availability of reliable industrial-scale data for lignin-based systems (Moretti et al., 2020a). Early-stage LCAs are thus mainly used to support technology development by identifying environmental hotspots and guiding potential improvements, although they are inherently more uncertain than assessments based on operational plant data, emphasizing the need for improved experimental validation and data management in future studies (Patel et al., 2012; Moretti et al., 2020b). For the need of scaling up foreground data, approaches generally include proxy-based methods, extrapolated data, formal calculations, and process simulation (Erakca

et al., 2024). Process simulations are presented as the most accurate approaches, but they can be time consuming (Piccinno et al., 2016). Classical engineering-based scale-up approaches are a simplest option relying on theoretical calculations derived from fundamental laws and empirical correlations. However, the impact of these approaches has not been compared under the same case study and the same conditions. In this regard, this work evaluates the extent to which simplified engineering-based scale-up methods can approximate simulation-based predictions, and by identifying the conditions under which their use remains valid for emerging, low-TRL technologies.

As mentioned before, process simulation is the most reliable, as it predicts system performance at larger scales, which is essential for fair comparisons with mature industrial processes (Ahmadi et al., 2019). The procedure typically begins with reconstructing and adapting the process flow diagram to define key unit operations followed by a simulation that enables detailed modeling, filling gaps such as energy use, often missing in low-TRL systems. From an LCA perspective, this ensures a consistent, complete inventory to support robust environmental assessment.

Systematic reviews on organosolv technologies in 2025 indicate that approximately 15 dedicated LCAs have evaluated organosolv pretreatment in lignocellulosic biorefineries, accounting for 20–30% of broader pretreatment LCAs (Tofani et al., 2023). Ryan et al. (2021) (Ryan and Yaseneva, 2021) reviewed 24 woody biomass conversion LCAs, including organosolv variants, highlighting an increasing of organosolv studies since 2010 due to favorable energy and toxicity profiles compared to other methods. Most organosolv studies applied LCIA methods based on ReCiPe (Moncada et al., 2018) on processes without energy integration, and used mass-based allocation, showing the effect of woody biomass on environmental performance. Earlier work by Prasad et al. (2016) benchmarked organosolv LCAs against alternatives, confirming scalability potential despite higher upfront energy.

The objective of this study is to assess the technical and environmental performances of a low-TRL organosolv fractionation process for lignin extraction, to support informed decision-making for future biorefinery developments. Patent data for the selected process (AST) were scaled-up using chemical engineering principles and process simulation, allowing the reconstruction and modeling of key unit operations, with different complexity levels. A software-based simulation approach and a simplified method based on chemical engineering rules were applied and compared. This approach, along with the parameter sensitivity analysis, generates a consistent large-scale Life Cycle Inventory (LCI), facilitating a robust and comparable LCA. Static, prospective (pLCA) and dynamic (dLCA) LCA are applied to the case study to reveal different facets of the system, and respond questions like: i) which process configuration performs the best, ii) which are the most influencing process parameters and which are the most relevant performance indicators, iii) how the future context influences the impact results, iv) is there a climate benefit for producing lignin by this technology.

2. Materials and methods

2.1. Design and simulation of Organosolv AST reference fractionation process at industrial scale (scenario AST)

This process is currently at a low TRL, with feasibility data available in several patents, but without complete mass and energy balances (Manesh et al., 2014; Manesh, 2014; Ali, 2014). Despite providing useful information on yields, solvent separation, and prospective estimates for higher lignin production rates up to 0.125 t per day, the descriptions in (Manesh, 2014; Ali, 2014) were insufficient to fully characterize the process performance, energy and solvent consumption, as well as key conversion and separation specifications when the process is envisaged within a specific industrial scale flowsheet. Experimental tests have been reported in (Manesh, 2014; Ali, 2014) on beech wood, corn stove, bark, grass and bagasse, however the composition of these raw materials was not provided.

The AST process employs a solvent composed of n-butanol and water, where n-butanol, assisted by sulfuric acid as catalyst, selectively dissolves lignin while preserving the structural integrity of the cellulose and hemicellulose fractions (Erakca et al., 2024). The process generates three main product streams:

- i. lignin-rich organic liquor phase containing dissolved lignin, residual chemicals, and butanol;
- ii. aqueous liquor phase composed of water and minor solubles;
- iii. solid pulp phase consisting of cellulose, hemicellulose, and ash.

The AST process demonstrates high adaptability to various lignocellulosic feedstocks while maintaining high product yields (Ali, 2014). Unlike conventional fractionation processes, which result in significant solvent losses, the low TRL AST process integrates a partial solvent recovery and recycling system to improve solvent efficiency, however, this is not sufficient to achieve a sustainable process.

As a first part of the methodology, based on the data and specifications provided from the low TRL patents (Manesh et al., 2014) the process has been scaled-up to reach a daily input of 0.5 tons of biomass, and to yield approximately 0.125 tons of lignin per day. A comprehensive process flow diagram (PFD) at this scale and associated simulation were developed in this work to accurately quantify mass and energy balances and specify performance indicators. Note that this scale of production is reasonable and can be theoretically extended to an industrial scale production following the same process flow diagram. Fig. 1 shows the PFD as designed and simulated with ProSimPlus® chemical process simulation software, using Simulis Thermodynamics® for the calculation of thermophysical properties and phase equilibria for pure components and mixtures. The main assumptions underlying the molecular definition of the components, as well as the reaction stoichiometries considered for the AST reference fractionation process, are detailed in Section 3 of the SI. The specifications for the main unit operations involved are gathered in Table S2 of the SI.

The composition of lignocellulosic feedstocks largely varies, but for the use in simulations, biomass with low moisture content (5.5 wt%) and a relatively high lignin content (25.7 wt%) was considered (Trubetskaya et al., 2016), suitable for achieving the daily lignin yield reported by (Manesh, 2014; Ali, 2014). The detailed composition of the lignocellulosic feedstock, akin to a hardwood composition, are provided in Table S1 of the SI.

As illustrated in Fig. 1, the process begins with biomass grinding and sieving. The biomass is fed at a flow rate of 20.83 kg·h⁻¹ which ensures the relative expected production of 125 kg lignin per day. Biomass enters at ambient conditions and is then grinded and sieved to reduce particle size and remove oversized fragments. Since ProSimPlus® does not include a module for mechanical operations an additional module was implemented to calculate the energy consumption by applying the equations and data provided in Section 2 of the SI.

In the fractionation stage, a batch high-pressure stirred reactor is considered where three components are introduced along with the pretreated biomass: n-butanol (organic solvent), sulfuric acid (catalyst), and water. Initially, butanol and water (added as a 1:1 mass ratio) are each fed at 52.08 kg h⁻¹, while sulfuric acid is introduced at 0.625 kg h⁻¹ (~0.6 wt% relative to the incoming liquid stream) (Manesh et al., 2014). This result in a liquid-to-solid ratio of 5:1 inside the reactor. The fractionation reactor operates for 90 min at 178 °C under pressure of 12 atm. Several reactions proceed simultaneously, including notably the solubilization and depolymerization of lignin into the organic phase, the partial hydrolysis of cellulose and hemicellulose within the solid pulp, and the formation of secondary compounds such as furfural and other dehydration products (Manesh et al., 2014) as shown in Table 2. The outlet stream from the fractionation reactor consists of:

- (i) Heterogenous liquor phase, which separates into two liquid phases due to the non-ideal behavior of the solvent-water-lignin

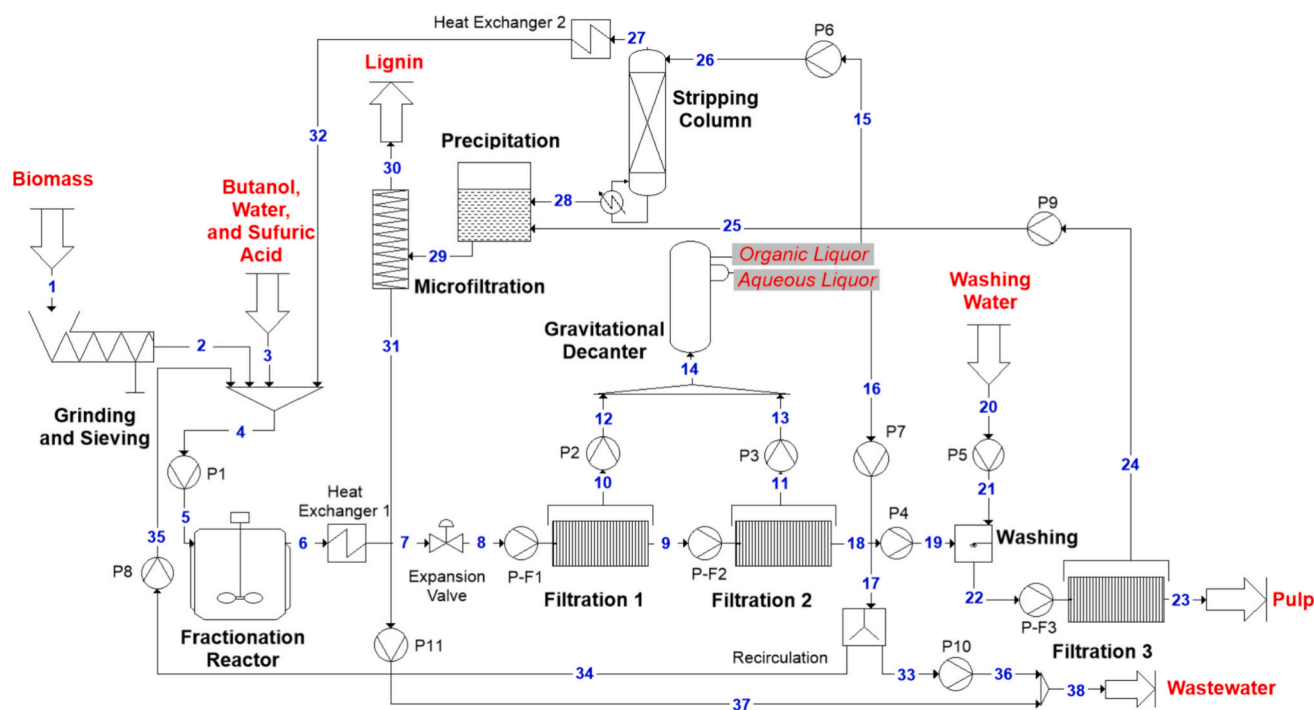


Fig. 1. Process flow diagram of the AST reference fractionation process using ProSimPlus.

mixture (Prausnitz et al., 1998): (a) an organic phase, enriched in n-butanol and dissolved lignin; it also contains reaction products such as furfural and C₆ sugars released from the extensive solubilization of hemicellulose (Manesh et al., 2014), (b) an aqueous phase, predominantly water, containing residual impurities, unreacted soluble components, and low concentrations of byproducts.

- (ii) Pulp phase, consisting of the remaining solid fraction, mostly cellulose, residual hemicellulose, ash, and small quantities of non-solubilized lignin.

The reactor pressure is set to 12 atm and the reaction medium is in the liquid state at 178 °C (Mesa et al., 2016). Although the mutual solubility of water and n-butanol increases markedly with temperature, the presence of dissolved lignin fragments and reaction products promotes liquid-liquid phase separation upon cooling and depressurization (Maneshi, 2014). Therefore, while the reactor operates in liquid phase under high-temperature and high-pressure conditions, phase splitting occur upon discharge, yielding the characteristic organic and aqueous liquor phases. Note that, the electrical power required for reactor stirring as well as the energy demand for microfiltration, were also estimated as described in Section 2 of the SI.

After cooling and expansion to 1 atm, the solid-liquid separation takes place consisting of two plate-frame filters operating in series (Filtration 1 and 2, Fig. 1): (i) first plate-frame filter: produces a pulp cake with 90% moisture content while 2.25% residual solids remain in the filtrate. (ii) second plate-frame filter: Reduces the cake moisture to 60%, solids remain in the separated liquor. Both filters operate at 8 atm and designed with the above-mentioned characteristics to ensure optimal lignin recovery. The resulted solid pulp stream is directed toward a washing step, using pure water injected at a flow rate of 52.08 kg h^{-1} , to remove excess butanol and residual liquor entrained with the pulp. After washing, the mixture of washed pulp and liquid exits the section at ambient temperature and pressure and is conveyed to a supplementary separation stage (Filtration 3, Fig. 1). In this step, the liquid is separated from the solid pulp using a plate-frame filter, yielding a pulp with 65% moisture and a filtrate with 4.5% residual solids.

The liquor streams are then mixed and fed into a gravitational decanter, which separates the liquor into two immiscible layers. Separation efficiency in the decanter is enhanced through temperature control at 15 °C. The aqueous liquor phase is recycled back to the pretreatment stage, with a purge fraction sent to an external wastewater treatment plant. The organic phase leaving the decanter is fed to a five-stage stripping column equipped with a reboiler operating at a vapor ratio of 0.9 relative to the feed flow rate. The stripper top stream, composed mainly of butanol and water at 109.6 °C, is sent to the feed tank. An important criterion is the presence of furfural in this recycled stream, over time. Furfural is generated directly from biomass and it functions as a self-sustaining solvent. This reduces the need for fresh butanol and can result in a surplus that is reused in subsequent lignin extraction cycles (Manesh et al., 2014). The stripper bottom stream consists of lignin and other dissolved chemicals, exiting the reboiler at 140 °C, and is sent to a precipitation tank that is facilitated using the washing liquid recovered from the pulp washing step, which contains residual butanol.

Precipitation is carried out at a ratio of 3 kg of water per 1 kg of solution, promoting lignin recovery as fine granulated particles (Smit et al., 2022). These are subsequently separated from residual chemicals in a microfiltration unit from which the outlet streams are a high purity lignin and a chemical-rich liquid. Lignin recovered as a granulated solid contains approximately 90% solids, 0.5–8% residual organic solvent, and moisture due to the hydrophobic nature of lignin (Microfiltration, Fig. 1). Lignin exhibits high purity (>80%), with 2–3% phenolic compounds and 1–1.5% ash.

The process illustrated in Fig. 1 is simulated under two contrasting energy scenarios, with and without heat integration, aiming to illustrate the energy gain by recovering residual heat from hot process streams and transferring it to cold streams through intermediate heat exchangers.

2.2. Modified AST fractionation process with enhanced solvent recovery (scenario AST-SR)

It is essential to recognize that solvent recovery, beyond lignin

production, constitutes a major focus due to its energy and cost implications. The AST process, as described, does not particularly prioritize solvent recovery as the focus is primarily on lignin production and yield (Manesh et al., 2014; Manesh, 2014). Moreover, a preliminary study, presented in Section 7.4 of Supplementary Information, demonstrated the large impact of butanol. Consequently, the AST process was modified as illustrated in Fig. 2 to incorporate an enhanced solvent-recovery strategy aiming at reducing markedly the amount of solvent used. The specifications for the main unit operations involved are gathered in Table S3 of the SI.

The original stripping column before precipitation was removed and a new 10-stage distillation column with a reboiler and condenser was introduced (distillation column, Fig. 2). The organic liquor from the decanter is now sent directly to the precipitation tank with the washing liquid. After precipitation, the stream exits and passes through the microfiltration unit to separate the solid lignin. The remaining mixture is further filtered through press filtration (plate-and-frame) to produce a cake with ~90% moisture, which is returned to the gravitational decanter.

In order to improve the solvent recovery two specific actions have been considered. First, the aqueous liquor leaving the gravitational decanter in Fig. 2 follows a slight purge of 5% at stream 41 (Fig. 2). Second, the liquid-solid suspension after washing in stream 22 enters first in a press filtration (plate-and-frame) to reach 60% cake moisture and the resulting cake passes through a more intense mechanical filtration using belt filters to reach a pulp with 40% moisture in stream 49.

The distillation column together with the above-mentioned enhanced filtration system allowed a marked recovery of 50 kg h^{-1} of butanol, reducing the fresh solvent requirement from 11.6 kg h^{-1} to 1.3 kg h^{-1} (i.e., 90% reduction in fresh solvent use). Literature on organosolv processes demonstrates that solvent recovery efficiencies of 90–97% are achievable through distillation and recycling systems. For example, ethanol-based organosolv industrial processes such as the Alcell technology have demonstrated solvent recovery efficiencies above 90–95% (Brosse et al., 2019; Lora and Glasser, 2002), while process simulation studies have reported recovery efficiencies up to 97% for solvent in organosolv systems (González et al., 2008). This behavior is consistent with fundamental separation principles and industrial distillation performance, where multistage columns routinely achieve high

separation efficiencies depending on operating conditions (Seader et al., 2010).

Most process water, particularly washing water, is also recycled. The column top stream, containing butanol and water is cooled in Heat exchanger 2 and then recycled. The bottom stream, composed of residual chemicals, is sent to water treatment. In addition, the wastewater stream, composed of dissolved xylose (C_5 sugars), requires further valorization, which lies beyond the scope of this study.

2.3. AST main settings for simulation and reactions involved

UNIFAC thermodynamic activity coefficient model was employed to account for non-ideal behavior in the liquid phase, including phase splitting and liquid-liquid equilibrium (Peres and Macedo, 1997). In terms of components, structurally analogous compounds were selected as proxies because several chemical species are not available in the standard database for molecular properties. Their thermophysical properties were adjusted accordingly, estimated or calculated using available methods (Rameshkumar et al., 2022), as summarized in Table 1. Additionally, complementary information on characterization of chemical components is provided in Table S4. Note that the chemical formulae were adapted to match stoichiometry in the reactions given in

Table 1
Component properties and proxy molecules used in modeling.

Name	Chemical formula	Proxy molecule	Adjustments
Cellulose	$\text{C}_6\text{H}_{10}\text{O}_5$	Glucose	Molecular weight: set according to chemical formula
Cellobiose	$\text{C}_{12}\text{H}_{22}\text{O}_{11}$	Glucose	Molecular weight: set according to chemical formula
Hemicellulose	$\text{C}_5\text{H}_8\text{O}_4$	Glucose	Molecular weight: set according to chemical formula
Lignin	$\text{C}_8\text{H}_{10}\text{O}$	Ethyl phenol	Molecular weight: set the MW of methyl phenol
Dissolved Lignin	$\text{C}_8\text{H}_{10}\text{O}$	Methyl phenol	Physical state at 25 °C: unknown (affected by the thermodynamic model)
Dissolved Xylose	$\text{C}_5\text{H}_{10}\text{O}_5$	Xylose	Physical state in aqueous solution: Completely soluble
Furfural	$\text{C}_5\text{H}_4\text{O}_2$	Furfural	Physical state in aqueous solution: Completely soluble

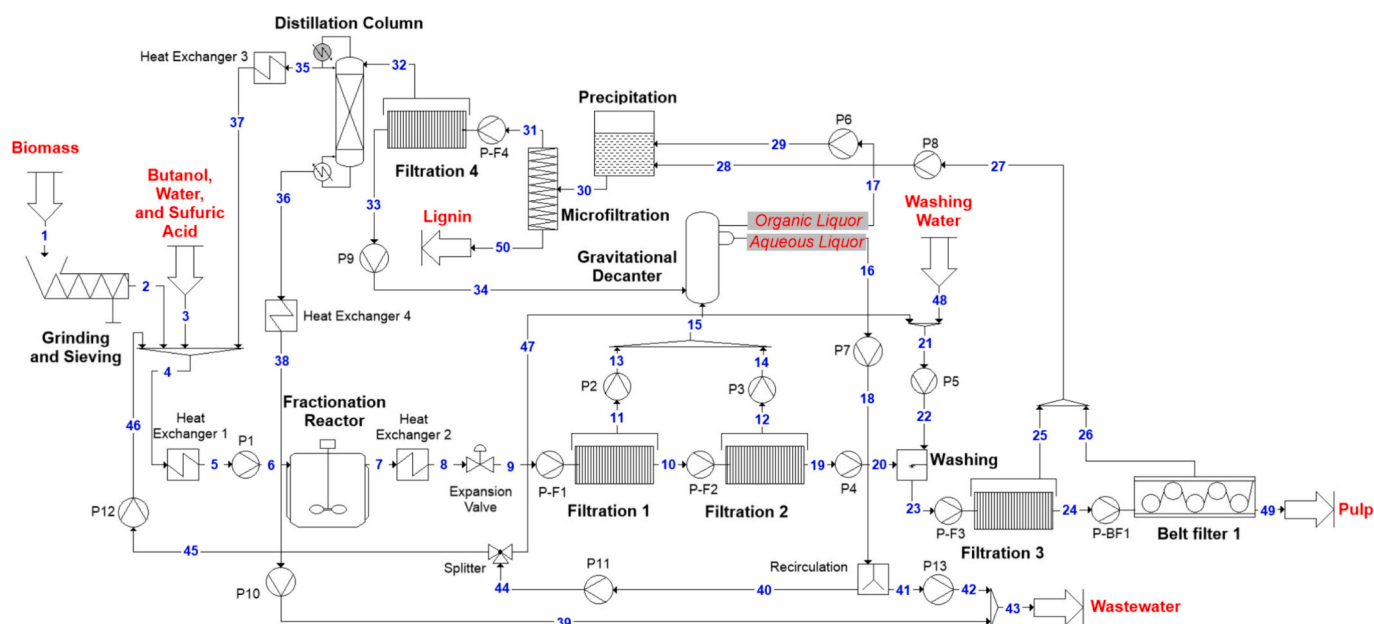


Fig. 2. Process flow diagram of the modified AST process with enhanced solvent recovery (scenario AST-SR).

Table 2

Main organosolv fractionation reactions and associated conversions (Aden et al., 2002).

Chemical reaction	Stoichiometry	Conversion
Dissolution of lignin	$C_8H_{10}O_{(s)} \rightarrow C_8H_{10}O_{(aq)}$	1
Hydrolysis of cellulose	$C_6H_{10}O_5 + H_2O \rightarrow C_6H_{12}O_6$	0.077
Depolymerization of cellulose	$C_6H_{10}O_5 + 0.5 H_2O \rightarrow 0.5 C_{12}H_{22}O_{11}$	0.007
Hydrolysis of hemicellulose	$C_5H_8O_4 + H_2O \rightarrow C_5H_{10}O_5$	0.925
Dehydration of hemicellulose	$C_5H_8O_4 \rightarrow C_5H_4O_2 + 2H_2O$	0.05

Table 2.

Lignin is composed by Guaiacyl (G), Syringyl (S) and *p*-Hydroxyphenyl (H) which correspond to phenolic structures similar to methyl and ethyl phenol. Hence, lignin and dissolved lignin were modeled using ethyl phenol and methyl phenol. Methyl phenol represents one of the core structural units of lignin, specifically the *p*-hydroxyphenyl (H) unit (Abdelkafi et al., 2011), and is water-soluble under ambient conditions. In contrast, ethyl phenol is less soluble, while other lignin-derived units such as syringyl, remain solid (Wang et al., 2021). Furthermore, the molecular weight of methyl phenol was applied to the dissolved lignin molecule to better capture its aqueous behavior. These phenolic monomers can represent lignin dominant intermolecular interactions (Méndez Seviliano et al., 2014) within the UNIFAC thermodynamic model which estimates predictively activity coefficients and phase equilibria for well-defined small molecules and cannot directly represent macromolecules such as lignin (Prausnitz et al., 1998).

In terms of reactions, the study focuses on five key reactions as detailed in Table 2. One primary reaction is the hydrolysis of hemicellulose by water, which produces xylose. Under elevated temperatures and the presence of acidic catalysts, a portion of xylose degrades into furfural. Similarly, cellulose undergoes hydrolysis to glucose, with cellobiose formed as an intermediate that can be subsequently converted to glucose (Manesh et al., 2014). Conversion rates were adopted from Aden et al. (2002) as the biomass composition in this study falls within a comparable range (Table S6), while Table S5 is the SI lists the potential secondary reactions.

Moreover, to reflect the actual energy requirements, the reaction enthalpy values in the simulation were adjusted based on literature data. Lignin, due to its complex polyphenolic structure, requires considerably more energy for dissolution than cellulose or hemicellulose. It consists of monolignol units connected by strong carbon-carbon and ether bonds, particularly the chemically resistant β -O-4 linkages. Cleaving these bonds is endothermic and typically requires elevated temperatures. The bond dissociation enthalpy of β -O-4 linkages, which concerns 60–70% of lignin, ranges from 196 to 323 kJ/mol depending on bond position and temperature (298–1000 K); a representative value of 200 kJ/mol was adopted for this organosolv process (Azad et al., 2020). In contrast, cellulose consists of highly ordered β -1,4-linked glucose chains that form extensive molecular hydrogen bonds, creating a stable crystalline structure. The enthalpy assumed for H_3O^+ -catalyzed hydrolysis of the β -1,4-glucan bond is -12 kJ/mol per glucose unit, consistent with literature values for the organosolv mode ranging from -18.46 kJ/mol to 0.03 kJ/mol (Ibbett et al., 2011). Hemicellulose, unlike cellulose, is amorphous, formed by branched heteropolymers composed of various sugar units, such as xylose. Hydrolysis, typically achieved via acid catalysis, targets the glycosidic linkages within the polymer. Reported enthalpy for hemicellulose hydrolysis ranges from 8.66 to 12.40 kJ/mol; a value of 11.5 kJ/mol was adopted in the organosolv process (Mukherjee et al., 2017).

2.4. Simplified alternative method for calculating material and energy flows (scenario AST-HC)

Simulations approaches need advanced modeling and simulation tools and are often complicated for LCA practitioners, especially for

evaluating emerging technologies. A complementary simplified method was applied to estimate the material and energy flows, based on physical laws and chemical engineering practices detailed in section 2 of the SI. This considers the main operations based on the flowchart of the process adapted from (Manesh et al., 2014) and provided in SI. In this configuration, the solvent is internally recycled after distillation (100% recovery), with 2% loss in filtration. This simplified method could be considered as an alternative to the simulation-based scenario AST-SR at the condition of acceptable errors.

2.5. Life Cycle Assessment

The environmental performance of lignin production from scaled-up AST organosolv process, as described in Sections 2.1–2.2 was evaluated using LCA. The LCA methodology was applied following the four phases as described in (ISO, 2006a; ISO, 2006b): (1) goal and scope definition, (2) life cycle inventory (LCI) compilation, (3) life cycle impact assessment (LCIA), and (4) result interpretation.

The functional unit is “the production of 1 kg of lignin” and the cradle-to-gate system boundaries is presented in Fig. 3.

The attributional approach was applied, with economic allocation using prices provided by (Fabiola, 2024) (900 EUR t^{-1} for lignin and 600 EUR t^{-1} for pulp), and shown in Table S10 along with the respective allocation factors.

2.5.1. Life cycle inventory and impact assessment

Background data were obtained from the Ecoinvent v3.9.1 database (Wernet et al., 2016), focusing on the European market and applying the cut-off system model. The foreground inventory for the scaled-up AST process from low-TRL was obtained using industrial scale process flowsheet building and simulation, as described in Sections 2.1–2.2, for AST and AST-SR scenarios with and without enhanced solvent recovery, and by simplified calculations for AST-HC (Section 2.4). The process is considered implemented in France, so LCA datasets were selected from Ecoinvent database prioritizing the French market when available, and the broader European market otherwise. Part of furfural is emitted in air, because it is volatilized from the alcohol-water solvent at high temperature, and, consequently, its presence in the aqueous phase is minimal (Köchermann et al., 2018).

The Environmental Footprint (EF) 3.1 method, recommended by the European Platform on LCA, was used to calculate the environmental impacts as it provides a harmonized set of 25 environmental impact categories (Nickel, 2022). The overall LCA implementation and scenario analysis were conducted using Brightway2, connected to Activity Browser, a Python-based tool (*‘Learn Brightway’ Book, 2024*). The ProSim simulations were connected with the LCA tool allowing an automated parametric analysis.

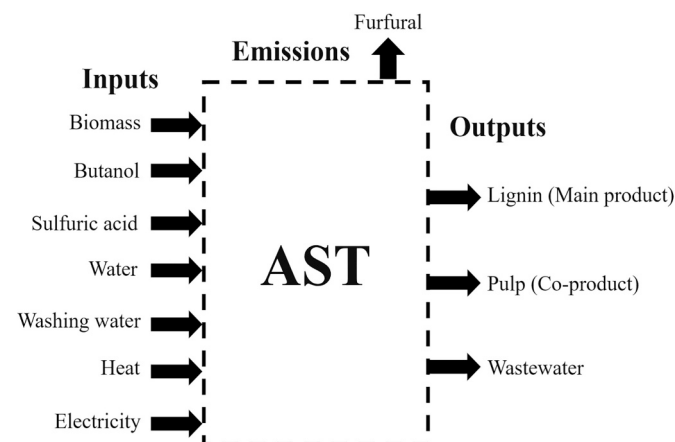


Fig. 3. Cradle-to-gate system boundaries for the organosolv lignin production.

2.5.2. Prospective Life Cycle Assessment (pLCA)

While most LCA studies implicitly rely on assumptions about future conditions, prospective LCA (pLCA) explicitly targets technologies at early stages of development. These technologies are often not yet commercially available and may exist only at low scales. In this context, an LCA is considered prospective when an emerging technology is assessed based on its expected future operation, typically assuming large-scale deployment under future, realistic market conditions (Nurdiawati et al., 2025).

Compared to conventional LCA, pLCA differs in both objectives and methodological choices, while it must explicitly address data shortage, higher uncertainty, and temporal inconsistencies between foreground and background systems (Tuomisto et al., 2022). Despite these challenges, pLCA provides valuable insights during early development phases, allowing environmental considerations to update technology design and scale-up strategies while key parameters remain flexible. However, many pLCA studies still rely on present-day background inventories, which are unable to capture future changes in energy systems, material supply chains, and technology deployment, leading to biased results (Arvidsson et al., 2018). To overcome this issue, recent approaches integrate future scenarios derived from Integrated Assessment Models (IAMs) into life cycle inventory databases. IAMs simulate long-term developments in energy use, land use, and emissions under varying socioeconomic and policy assumptions (*What are IAMs? – IAMC*, 2007). Tools such as *premise*, an open-source Python-based tool, apply a set of transformations to energy-intensive activities in the ecoinvent inventory database based on projections derived from IAMs (User Guide, 2025). These tools enable the systematic integration of IAM outputs, such as those from REMIND, which combines macroeconomic growth, energy system transitions, and climate policy analysis, and IMAGE, which provides a comprehensive representation of long-term interactions among human development, energy demand, land use, food systems, and environmental change, into the ecoinvent database. This integration allows the generation of time-resolved prospective life cycle inventory (LCI) databases, thereby improving the robustness and consistency of prospective Life Cycle Assessment (pLCA) results (Sacchi et al., 2022; Kimita et al., 2021).

In this work, the chosen scenario is “Remind-SSP2-NDC”, which is built on the Shared Socioeconomic Pathways (SSP) and based on the Nationally Determined Contributions (NDC). The REIMIND scenario simulates how regions invest in different technologies and energy resources to balance economic growth and climate targets while considering factors like energy efficiency, emissions and resource availability (Baumstark et al., 2021; Nurdiawati et al., 2025). The use of SSPs helps to cover uncertainties regarding technological development for renewable energy or fossil fuel availability but also social and behavioral development like population growth. In order to take a moderate climate target, a 2 to 2.5 °C increase on temperature in 2100 has been considered.

2.5.3. Dynamic Life Cycle Assessment (dLCA) for climate change impact

The bio-based systems involve CO₂ capture by the biomass and CO₂ emissions from the biological system and from the economic activities. It is now acknowledged that static LCA cannot capture the complexity of carbon capture and emission dynamics and its effect on global warming (Tirut-Barna, 2021). Unveiling the biomass potential for climate change mitigation needs adapted approaches like the dynamic LCA (dLCA). Here, the greenhouse gas emissions and carbon capture are considered following the methodology described in (Tirut-Barna, 2021) with the CCI-tool calculator (*Climate Change Impact Tool*, 2024) for the dynamic climate change impact. The dynamic inventory was built up from the LCI of AST-SR scenario, by positioning the processes on a time scale. Then, global mean temperature change (GMTC) and cumulated radiative forcing (IRF) indicators were calculated in function of time. The background principles, mathematical development and parameters of the dynamic impact calculation were presented in detail

in (Tirut-Barna, 2026). The temporalized inventory (emissions positioned at different moments on the timescale) is combined with transient response from the climate system (including substance fate in environment and thermal balance) via impulse response functions provided by IPCC.

In order to capture the whole carbon cycle and its effect on climate, and the trade-off between carbon capture and greenhouse gas emissions in the manufacturing step, the time scale covers the whole life cycle (cradle-to-grave), from tree plantation, harvesting, processing and lignin production, as well as the use phase and end of life of lignin. Lignin is considered here as curing resin for wood panels, with a lifetime of about 20 years. Two end of life cases are considered: i) incineration at year 20 with all carbon emitted as CO₂, and ii) recycling with incorporation in a new product for 20 years, followed by incineration at year 40. There are no emissions during the use stage, and the only emissions at the end of life come from lignin burning.

2.6. Parametric, Pearson correlation and uncertainty analysis

One-at-a-time (OAT) parametric analysis was performed on AST-SR scenario, by varying selected input parameters individually by $\pm 5\%$ and $\pm 20\%$, of their initial values (Groen et al., 2014). The target parameters were selected based on their influence on overall system efficiency. These parameters are presented with their initial values and the tested deviation values in Table S9 of the SI. The effects of parameter variations encompassed most unit operations; however, the analysis focused on 9 key performance criteria: lignin and pulp yield, butanol and water input, reactor heat requirement, distillation heat consumption and the total process electricity consumption, heat and cooling demand. A Pearson correlation analysis (Schober et al., 2018) was applied to the performance indicator results, normalized to the functional unit of 1 kg of lignin produced, to quantify the relationships between parameters. Correlation coefficients were classified as strong ($|r| \geq 0.50$), moderate ($0.30 \leq |r| < 0.49$), weak ($|r| < 0.29$), or none ($r = 0$) (Saltelli, 2008). A Principle Component Analysis (PCA) (Jolliffe and Cadima, 2016) was also performed to confirm and strengthen the interpretations derived from the Pearson analysis (Abdi and Williams, 2010). This analysis was conducted first on the environmental impact indicators, and then on the main process-related performance criteria. Moreover, an uncertainty analysis was performed to assess the range of possible outcomes due to uncertainties in key inputs and assumptions (Sheikholeslami et al., 2023).

3. Results

3.1. Simulation results for AST fractionation process

The AST process flow diagram for lignin production and related simulation after scale-up, as described in Section 2.1, has been built and set to reach the same level of performance in terms of conversion and yield when the process is envisaged at an industrial scale. Table S7 of SI presents the simulation results for the reference process illustrated in Fig. 1. The main performance indicators from the process scale-up and simulation were verified against those estimated from patent including (i) Overall lignin yield (%), (ii) solid pulp yield (%). According to lignin yield, the patent specifies an overall lignin yield of 97.3%, while the simulation indicated 98.3%, corresponding to a deviation of 1%. Meanwhile, solid pulp yield (relative to the initial solids: cellulose, hemicellulose, lignin, and ash) was reported as 21.06% in the patent, against the simulated pulp yield of 20.83%, corresponding to a deviation of 1%. For a basis of 20.83 kg h⁻¹ of biomass treated, the system's energy consumption was evaluated based on the presence or absence of heat integration. Pinch analysis identified opportunities for heat recovery by exchanging heat between hot and cold process streams and indicated that 5.5 kW of thermal energy could be recovered, with a pinch temperature of 134 °C. Electricity demand remained constant at 1.44 kW in

both cases. As a result of heat integration, thermal utility requirements were reduced, with heating demand decreasing from 45.1 kW to 39.6 kW and cooling demand from 42.1 kW to 36.6 kW.

Energy consumption estimated by the simulation falls within normalized data from the literature, as given in Table 3, involving the core organosolv stages: pretreatment, fractionation, filtration, precipitation, separation, and purification. Here, electricity and heating energy were considered together by lack of more detailed literature data.

3.2. LCA results and interpretation

3.2.1. Life cycle inventory results

Based on the simulation results for AST reference fractionation process (Fig. 1 and Table S7) and for the modified AST-SR with enhanced solvent recovery (Fig. 2 and Table S8), LCIs were established and harmonized in Table 4, relative to the function unit (FU) of 1 kg lignin produced, with corresponding relevant data set from Ecoinvent 3.9.1. In addition, the inventory results from the simplified calculation method (AST-HC) were reported in Table 4.

The process with enhanced solvent recovery consumes significantly less solvent as expected, but also much less washing water. In contrast, it consumes more heat and sulfuric acid. However, the variability of the biomass composition could induce a variability in the process material and energy balance, which will be further explored in Section 3.3. Concerning the simplified method, the inventory diverges especially for the biomass input (as a result of a simplified mass balance), for sulfuric acid and water due to non-consideration of complex recycling. Heat demand is situated between those of AST and AST-SR scenarios because of simplified consideration of distillation operation. Moreover, the solvent recovery by distillation was considered complete, which is not the case in real operation.

3.2.2. Environmental impact results

The environmental impact results, normalized with respect to the highest value in each category, are shown in Fig. 4, for the three scenarios. These results considered economic allocation. It is observed that when the enhanced solvent recovery is implemented, the impacts decrease markedly with respect to the reference scenario in most categories by more than 60%.

Fig. 5 illustrates the contribution of different processes to three impact categories, chosen here for their distinct behavior: Climate change, global warming potential (GWP₁₀₀), Marine eutrophication: nitrogen (N), and Ionising radiation: human health, human exposure efficiency relative to u235 (u235). The complete set of results is provided in section 7.3 (Fig. S2) of the SI. According to Fig. 5, implementing solvent recovery in AST process substantially reduces the solvent-related emissions. In GWP₁₀₀ category, these emissions decrease from 2.7 to 0.5 kg CO₂-eq, while the heat-related emissions rise from 0.5 to 1 kg CO₂-eq due to the higher heat consumption. A detailed study of the environmental impact of the organosolv solvent used, based on the production pathways and effect on GWP₁₀₀, is presented in section 7.4 of the SI: producing 1 kg of 1-butanol generates 2.603 CO₂-eq.

Marine eutrophication impact (Fig. 5 – N) is generated by the solvent production, fossil fuels used for heat consumption and by the waste water treatment process. Electricity in this study was modeled using the dataset “Electricity, medium voltage, market for electricity in France,”

Table 3

Energy consumption range of the AST reference fractionation process compared with the literature (heat and electricity).

Energy consumption kWh/kg biomass	AST	Literature	Reference
With heat integration	1.96	1.11–2	(Moncada et al., 2018; Mesa et al., 2016; Viell et al., 2013; Kravanja et al., 2013; Nitzsche et al., 2016).
Without heat integration	2.23	2.1–3.29	

Table 4

Inventory table for the AST lignin production: AST reference fractionation process (AST), enhanced AST process with solvent recovery (AST-SR), simplified calculation method (AST-HC); without allocation.

	AST reference fractionation process (AST)	AST process with enhanced solvent recovery (AST-SR)	Simplified calculation method (AST-HC)	
Inputs	Inventory per kg of lignin produced			Ecoinvent 3.9.1- Cuttoff data set Wood chips production, hardwood, at sawmill, [Europe without Switzerland] 1-butanol, Hydroformylation of propylene, [RER] Sulfuric acid, Market for Sulfuric Acid, [RER] Tap water, Market for tap water, [Europe without Switzerland] Tap water, Market for tap water, [Europe without Switzerland]
Biomass	4.02 kg	3.93 kg	4.67 kg	
Butanol	2.21 kg	0.25 kg	0.27 kg	
Sulfuric Acid	0.05 kg	0.12 kg	0.14 kg	
Water	0.96 kg	0.80 kg	9.40 kg	
Washing Water	9.90 kg	1.38 kg	11.67 kg	
Utilities ^a				
Electricity	0.28 kWh	0.29 kWh	0.31 kWh	
Heat	27.12 MJ	39.78 MJ	33.16 MJ	
Output	Inventory per kg of lignin produced			
Pulp	1.97 kg	2.10 kg	2.33 kg	Ecoinvent 3.9.1- Cuttoff data set Wastewater, average, treatment of waste water, average, wastewater treatment [Europe without Switzerland]
Waste	(–)0.0141 m ³	(–)0.0033 m ³	(–)0.0217 m ³	
Water				
Lignin	1	1	1	Biosphere3 Furfural, Air
Emission				
Furfural	0.0003	0.0132	0	

^a Utilities are given by considering the heat integration in the process.

composed of 99% medium-voltage electricity sourced from a high-voltage mix containing 71.3% nuclear power, 18% hydropower, and only 3.7% natural gas combined-cycle. The dominance of nuclear power is visible in Fig. 5 – u235, for the ionising radiation, with an important contribution of solvent fabrication and of the direct electricity use in organosolv process. Most of the remaining 21 impact categories show the important contribution of the solvent and heat production, except for: acidification with important contribution of the catalyst (sulfuric acid), biogenic GWP₁₀₀ and land use - soil quality index, with biomass as main contributor. Wood chips are used as feedstock in these processes, and their production, transport, and handling influence the overall footprint.

Comparing the LCA results for AST-HC, i.e. the simplified calculation approach of LCI, shows variations between –50% and 63% with respect

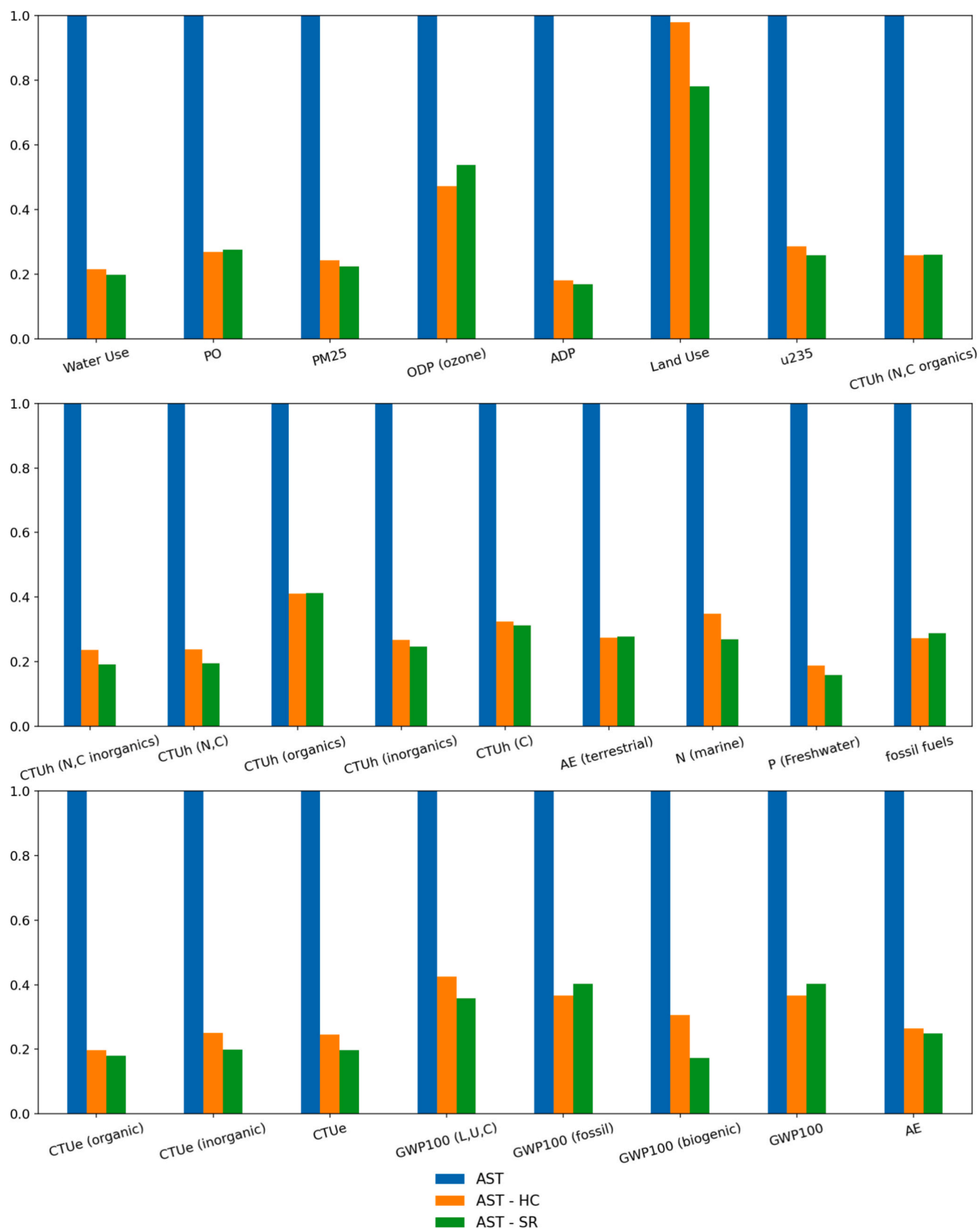


Fig. 4. Comparative results on environmental impact assessment: (i) AST reference fractionation process, (ii) modified AST fractionation process with enhanced solvent recovery AST-SR, (iii) simplified calculation method AST-HC (the sub-annotations of the impact assessment methods are presented in the list of acronyms and Table S11 of the SI).

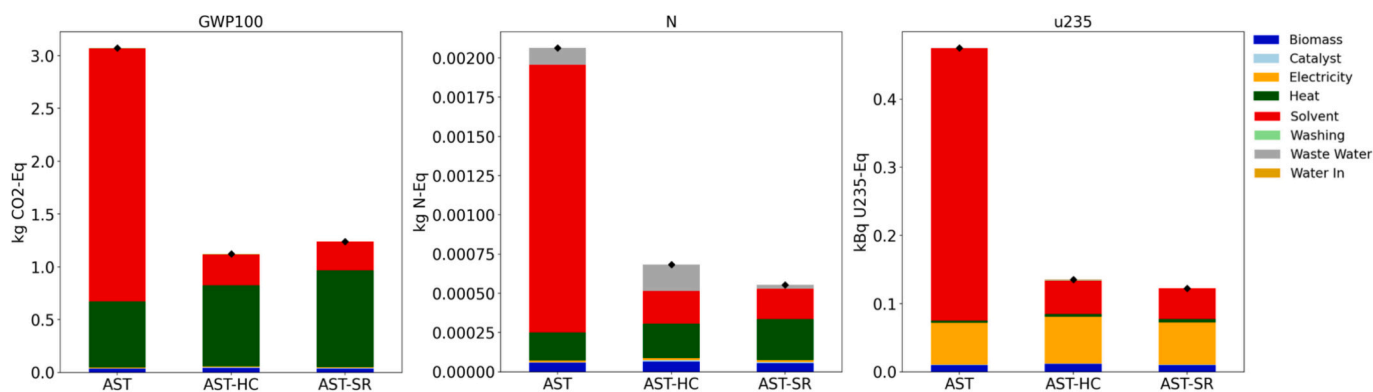


Fig. 5. Comparative contribution analysis of environmental impacts for the three scenarios studied: Climate change, global warming potential (GWP₁₀₀); Marine eutrophication: fraction of nutrients reaching marine end compartment (N); Ionising radiation: human health, human exposure efficiency relative to u235 (u235).

to AST-SR approach (impact results listed in Table S12). The most significant differences occur for ecotoxicity freshwater organics (CTUe (organics)), climate change biogenic (GWP₁₀₀ biogenic), and water use. If the ecotoxicity is underestimated (−50%) because various chemicals present in the waste water were not included in AST-HC, water use is overestimated (+50%) in AST-HC because of difficulty of accounting for internal recycling loops. Climate change GWP₁₀₀ is underestimated only by 8% and this is due to approximations in heat consumption. Moreover, overestimating the biomass input determines higher impacts in those categories highly influenced by the wood chips production, as mentioned above. These results indicate that the simplified inventory calculation method is suitable for preliminary estimations; however, when optimized internal recycling is needed, a simulation-based approach becomes necessary.

3.2.3. Prospective LCA results based on the future evolution of transport and energy systems

Prospective LCA results reflect the effect of electricity mix changes and transports by 2050, as included in premise tool. Fig. 6 reveals a progressive decrease in climate change impact over time primarily driven by the electricity production. In addition, 1-butanol contribution decreases with time due to the energy sources used for solvent production (Table S13). The decrease in electricity-related GWP over time is directly linked to the evolution of the electricity production mix under the SSP2-NDC scenario. In the early years, the electricity mix still includes a small but non-negligible share of fossil-based generation, such as natural gas combined-cycle power plants, accounting for approximately 3.5% of total electricity production. Toward 2050, the electricity

system undergoes gradual decarbonization in line with Nationally Determined Contributions and becomes increasingly dominated by low-carbon sources, primarily nuclear (approximately 70%) and hydro-power (around 38%), also characterized by a low carbon footprint (Market for electricity, medium voltage, 2024). Further reductions in electricity-related GWP₁₀₀ are limited, not due to technological constraints, but because the electricity system has already largely completed its transition toward low-carbon generation. In contrast, the mineral resource depletion (ADP) impact shows a progressive increase in time due to the energy production shift from fossil carbon to nuclear and renewable, requesting important infrastructures and metal consumption.

The same is observed for land use impact, due to the larger surfaces required by renewable energy production, as shown in Fig. S3. The observed increase of human toxicity (inorganics) (CTUh) is also due to this mineral consumption increase. The rest of impact categories show rather a progressive decrease in time.

The evolution of economy in prospective scenarios is managed internally in the integrated assessment models (IAM). For our case, the REMIND-NDC-SSP2 scenario already considers future changes in macroeconomics regarding electricity, transport changes are already included. Concerning the products, however, the use of economic allocation introduces substantial uncertainty, as future price estimations may not reliably represent the actual value of co-products. However, when the innovation is integrated into an existing and well-established market, such as the lignin market, the uncertainty associated with future prices can be partially reduced by referencing current market conditions, thereby making economic allocation a more appropriate and

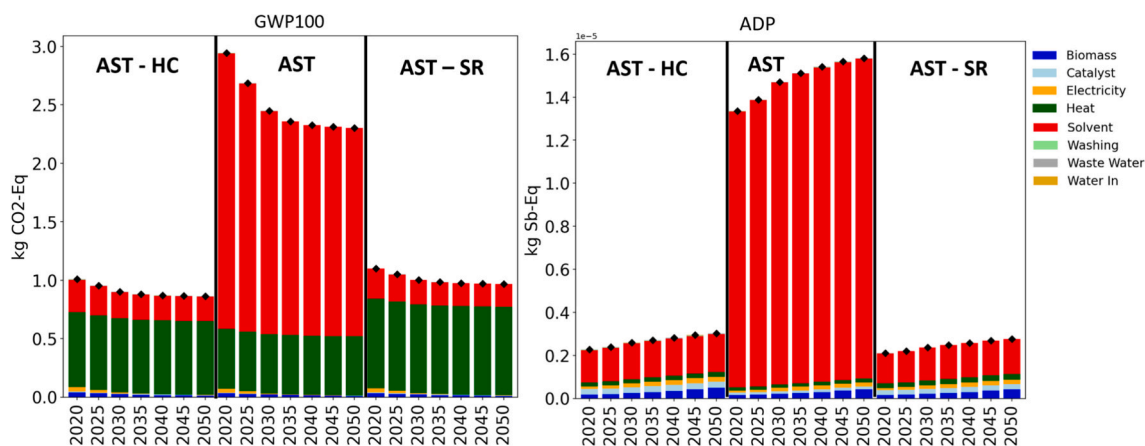


Fig. 6. Climate change impact (GWP₁₀₀) and mineral resource depletion (ADP) for the three scenarios in prospective LCA from 2020 to 2050 (all results are presented in section 7.5 of the SI).

representative method (Cucurachi et al., 2022). These results assume that the economic allocation remains constant in future scenarios, implicitly suggesting that market evolution for lignin and pulp follows the same proportional trend. However, an uncertainty analysis was conducted based on current price ranges to evaluate its impact, as reported in Section 3.3.3 and Section 8.2 of the SI.

3.2.4. Dynamic LCA

Beech was considered as the tree species for biomass feedstock (the major component of the wood chips dataset from ecoinvent 3.9), with a rotation time of about 140 years. First tinning of trees for logs and woodchips as byproduct production, can be made at 40 years (Deckmyn et al., 2004). The CO₂ capture dynamics by *Beech* tree was calculated with the Chapman-Richards model, as detailed in SI (section 7.6).

In the dLCA approach, the time zero can be placed anywhere on the timescale; here it was considered at the start of lignin utilization. The inventory was distributed on the timescale with a timestep of 1 year. On the timeline, CO₂ capture from atmosphere by trees starts at year -42 (in the past), wood harvesting (with the associated processes) is placed at year -2, and the whole lignin production activity is considered within the year -1. The end of life occurs at year 20, or at year 40 if one recycling loop is included.

Fig. 7 presents the calculation results for the two dynamic indicators for climate change impact, i.e. GMTC and cumulated radiative forcing (iRF, W yr·m⁻²), and global mean temperature change (GMTC, K), for the life cycle of 1 kg lignin produced in AST-SR scenario. To better unveil the influence of different life cycle stages, forestry (including tree growth and harvesting), biorefinery (AST-SR), and end of life incineration, were shown separately in Fig. 7, for both indicators, along with the total net result (black curves).

The net cooling effect of CO₂ capture in forestry activity is partially counterbalanced by greenhouse gas emissions from the organosolv process, but the net result still remains in the negative domain, i.e. net cooling effect on climate, until the lignin incineration, whensoever end-of-life takes place. The biorefinery emissions seem to not completely compensate the benefit of carbon capture in trees. In contrast, the end-of-life (incineration) will cancel this benefit by emitting the ancient captured carbon in wood. Fig. 7 – GMTC clearly demonstrates the temporal carbon storage effect on global warming (cooling effect) during the use stage of the lignin material, and the switch toward a warming effect after end-of-life. Fig. 7 – iRF, in contrast, shows that the net cumulated radiative forcing remains negative over long-term, which disagrees with the static LCA results. The climate change impact of AST-SR is 1.2 kg CO₂-eq, as provided in Section 3.2.2, for the cradle-to-gate system. If the use stage and end-of-life are added for the cradle-to-grave system, the result doesn't change because there are no emissions in the use stage and the incineration produces biogenic CO₂, which is considered with zero contribution in static LCA. Note that climate change impact in static LCA (GWP100) is calculated with iRF at 100 years divided by iRF100 of CO₂. However, the black curves indicate a negative

impact, as if the system had negative net emissions over a time horizon of 100 years (and more). This discrepancy is due to the fact that static LCA neither include the dynamics of biogenic carbon emissions/captures, nor the temporal carbon storage effect.

3.3. Key findings from parametric analysis, Pearson correlation, PCA and uncertainty analysis

3.3.1. Joint discussions on Pearson analysis and PCA

Pearson correlation analysis was applied to the nine performance indicators introduced in Section 2.6 as well as to the 25 environmental impact categories of the EF v3.1 method (Table S11, SI) in order to quantify the relationships among these indicators. Strong interdependencies were observed among the EF indicators supporting the selection of GWP₁₀₀ as a representative proxy for overall environmental performance. GWP₁₀₀ was selected as the primary environmental indicator due to its widespread international acceptance and policy relevance, as it is the default metric recommended by the Intergovernmental Panel on Climate Change (Intergovernmental Panel on Climate Change (IPCC), 2023; U.S. Environmental Protection Agency - GWPs, 2023) for comparing greenhouse gas emissions, and it is consistently adopted in major assessment frameworks such as the European Commission Environmental Footprint (EF 3.1) method (Andreasi et al., 2023). The latter was also pointed out and confirmed using a parallel independent PCA over the 25 environmental indicators of the EF v3.1 method (Fig. S4, SI).

The analysis further revealed that, with the exception of the quantity of fresh water input whose behavior is primarily governed by internal water circulation, most process parameters exhibit strong linear correlations with system performance. When normalized to the functional unit of 1 kg of lignin produced, lignin yield and total cooling energy demand showed strong negative correlations with most of the parameters, whereas pulp yield, butanol input, reactor heat duty, distillation heat consumption, total electricity use, and total heat demand were strongly and positively correlated with each other. Strengthened by a parallel PCA analysis, as illustrated in Fig. S5 (SI), this structure highlights three distinct groups of performance indicators: (i) a coupled set of energy and conversion-related indicators, (ii) a second group tightening lignin yield and cooling, and (iii) a third involving butanol and water input, which behaves largely independently due to process-internal recycling constraints.

As mentioned above, PCA was performed to confirm and consolidate trends illustrated through Pearson analysis. First PCA applied to the EF impact categories revealed that the first principal component captures the dominant variance associated with energy-related burdens, explaining the strong coherence among impact categories and justifying the use of GWP100 as a robust environmental descriptor. A second PCA conducted on the process performance indicators showed that the first principal component is primarily driven by energy related indicators - heat and electricity - opposed to lignin yield, reflecting a trade-off between process intensity and product recovery. The second principal

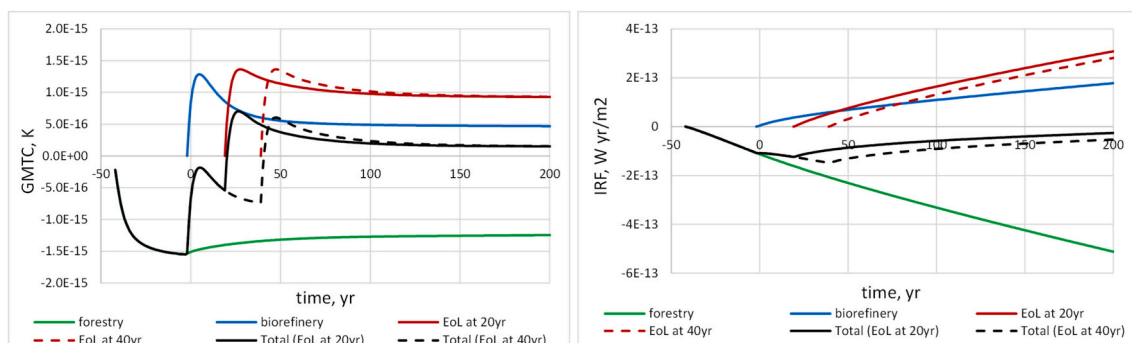


Fig. 7. Dynamic LCA results (cradle-to-grave): global mean temperature change (GMTC) and cumulative radiative forcing (iRF) in function of time.

component is largely associated with water input confirming its relative independence from the main energy–yield trade-off identified in the system. Beyond confirming the Pearson correlations PCA provides a physical interpretation of the system behavior: the dominant axis represents an “energy intensity versus yield efficiency” gradient, where higher energy consumption is associated with lower lignin recovery per functional unit, while the secondary axis reflects water and solvent management strategies largely decoupled from the core thermochemical performance.

Based on the classification of correlation coefficients as strong ($|r| \geq 0.50$), moderate ($0.30 \leq |r| < 0.49$), weak ($|r| < 0.29$), or null ($r = 0$), and supported by a complementary Principal Component Analysis (PCA) (Mishra et al., 2017), the set of main performance indicators was reduced to four (Fig. 8): lignin yield, water input, total heat demand (energy criterion) and GWP100 as the environmental indicator. Global Warming Potential GWP100 exhibited a strong negative correlation with lignin yield, a strong positive correlation with total heat demand, and only a weak correlation with water input, confirming its dependence primarily on energy-related process drivers.

3.3.2. Parametric analysis results

Moreover, parametric analysis on the 20 main design and operating parameters allowed the identification of their respective influences. The results of the parametric analysis are summarized in Fig. 9 as it is shown that all six performance indicators in this figure are driven mainly by the raw biomass composition, the lignin dissolution rate as well as the efficiency of the liquid-solid filtration steps. According to Fig. 9, lignin yield is primarily driven by biomass composition, more specifically by the initial lignin content of the raw biomass and the lignin dissolution conversion rate. The higher the lignin content, the higher lignin yield can be achieved, illustrating the overall efficiency of process for lignin extraction and purification. Regarding the pulp yield, an opposite effect can be observed compared to the lignin yield. That is to say, the pulp yield would naturally decrease while increasing the lignin yield by increasing the lignin content of raw biomass with enhanced lignin dissolution.

The composition of biomass, particularly its lignin content,

modulates these relationships as a higher lignin content increases lignin yield and energy need, but leading to lower emissions. In contrast, lower lignin content elevates the solvent-to-lignin ratio, thereby increasing environmental impacts including climate change.

The moisture content of the filter cakes exerts a dominant influence on solvent use, required water input as well as energy need and GWP100 that represents the overall behavior of environmental footprints. Filtration 3 with the belt filter, represents the final solid–liquid separation step prior to solid pulp production (Fig. 2) and receives the largest water input from feed and washing streams. Consequently, it strongly affects pulp yield as well as the partitioning of water in the system. Filtration 5 (Fig. 2), on the other hand, located immediately upstream of the distillation column, is critical because its output partially feeds the decanter, where it mixes with previously separated aqueous and organic phases. Elevated cake moisture in Filtration 5 increases the liquid volume relative to dissolved lignin, thereby reducing lignin yield. Conversely, lower cake moisture directs a greater amount of solvent and water to the distillation column, enhancing lignin yield but also raising total energy consumption.

The operation of the distillation column, especially the liquid distillate flow rate, interacts with these filtration steps. Variations in the distillate flow influence the extent of water recycling, which in turn affects fresh water demand. However, the butanol-to-water ratio remains constant based on (Manesh et al., 2014), ensuring process stability. Fresh butanol reinjection is likewise ruled by filtration performance and the recovery ratio achieved in the wastewater treatment section as lower recovery ratios increase solvent demand, thereby elevating both energy consumption and GWP100 impact. The purge system was explicitly included due to its significant contribution to mass removal from the process, the resulting wastewater streams were identified and their treatment included in LCA.

3.3.3. Uncertainty analysis

Economic allocation was applied in accordance with ISO 14044 guidelines, which recommend allocation based on the relative economic value of co-products when physical relationships are not appropriate (ISO, 2006b). The initial price assumptions were provided by an

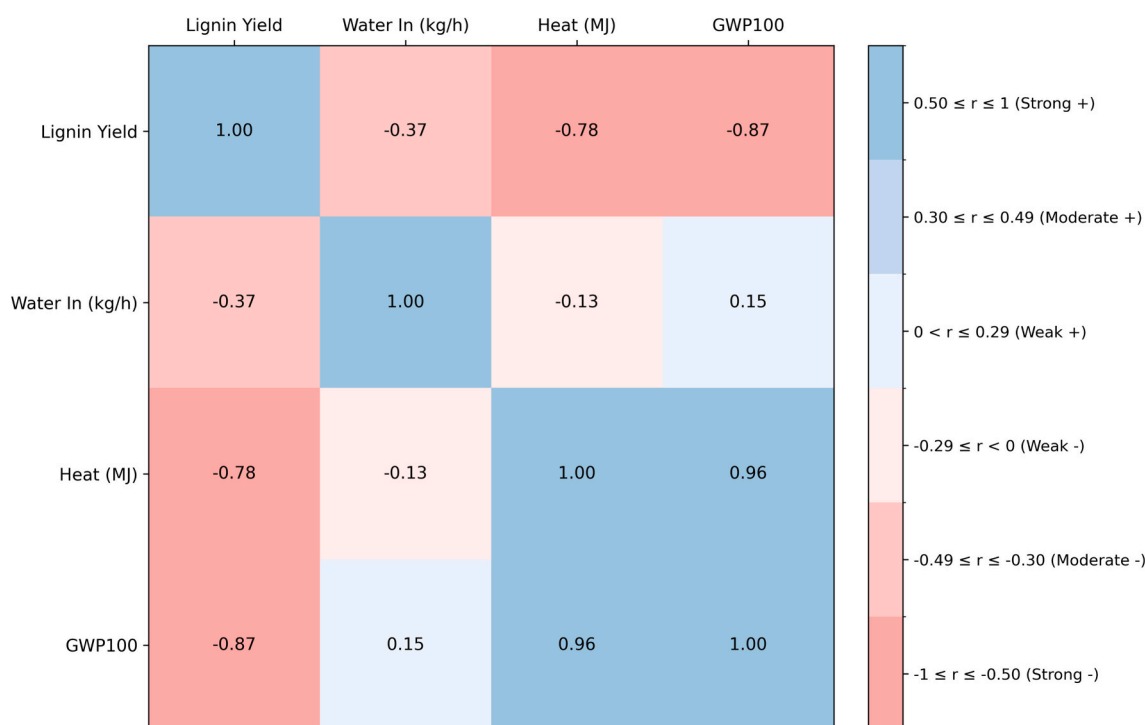


Fig. 8. Reduced set of representative indicators: three process parameters and one environmental impact category.

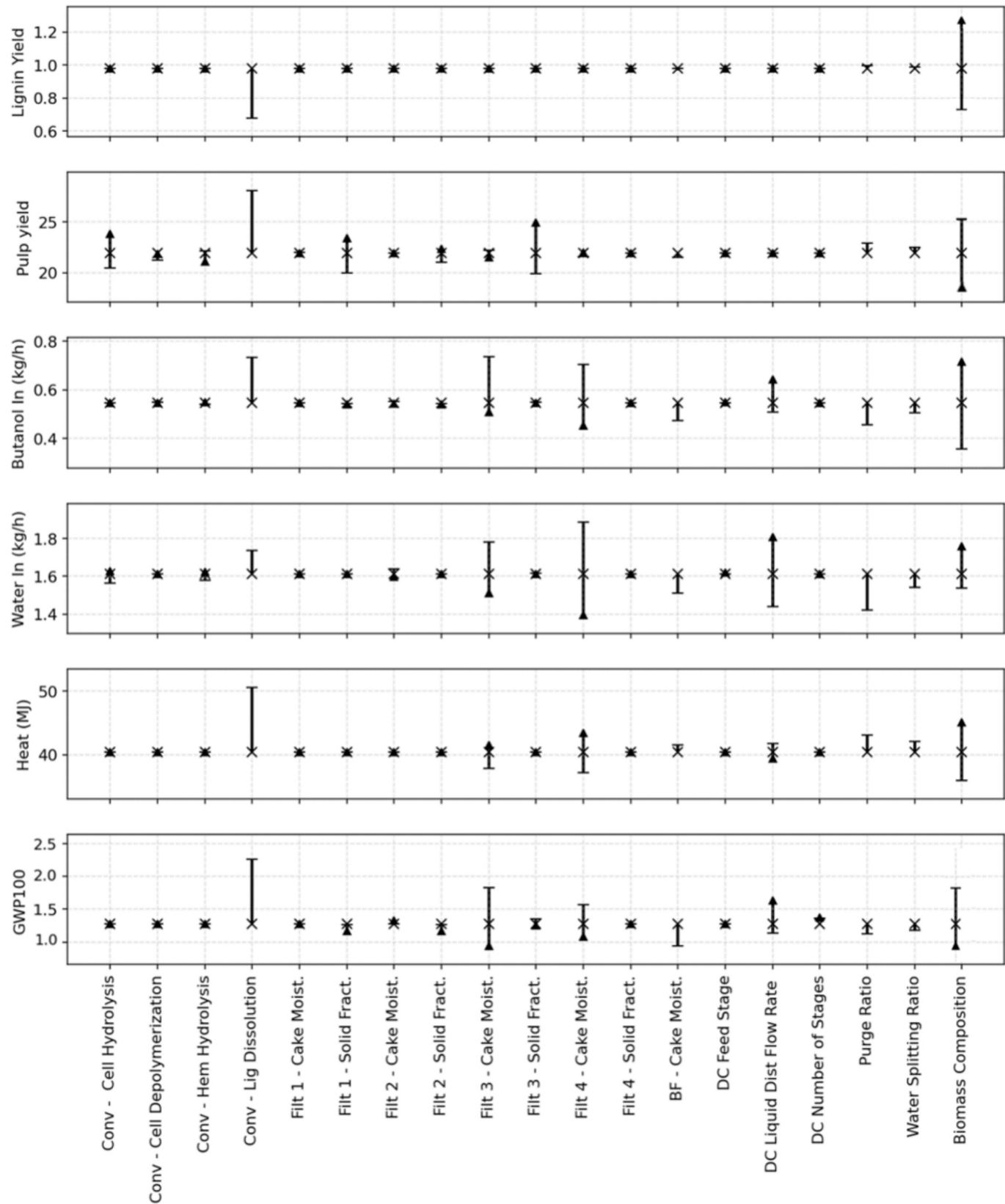


Fig. 9. Process indicators as functions of process parameters: results for maximum (▲), minimum (—), and reference (x) parameter variations.

industrial partner; however, the market prices of both lignin and pulp can vary significantly, leading to uncertainty regarding their impact on process performance. Lignin prices reported in the literature span within a wide range depending on the targeted application, from approximately 100 €/t for energy applications (typically associated with kraft lignin used as a fuel substitute (Mörck et al., 1988)), while organosolv lignin, due to its higher purity and added value, typically starts at around 450 €/t and can reach over 1000 €/t for high-value materials (Rinaldi et al., 2016; Kautto et al., 2014). Whereas, for cellulosic pulp, market data indicate typical prices ranging between 500 and 900 €/t (Nyman, 2026; Wood Pulp IndexMundi, 2026). In order to test uncertainty on economic allocation, two combination of extreme market price conditions were tested: the maximum lignin price combined with the minimum pulp price, and vice versa (i.e., minimum lignin price combined with maximum pulp price). The tested combinations are reported in Table S14 of the SI. Specifically, a low lignin price leads to an economic allocation factor of approximately 0.2, whereas a high lignin price results in a factor of about 0.5. Results are presented in Fig. 10 and are compared to the reference allocation factor of 0.43. It is observed that a lower allocation factor (0.2) results in a decrease of around 50% in emissions attributed to lignin, while a higher allocation factor (0.5) leads to an increase in impact value attributed to lignin. This demonstrates the strong sensitivity of the results to the economic allocation approach and confirms that allocation choices represent a key source of uncertainty in the LCA (Ekvall and Finnveden, 2001). Additional details are provided in Section 8.2 of the SI.

One of the main variables identified in the parametric analysis as significantly influencing process performance was the biomass composition, particularly the lignin content. A lower lignin content resulted in higher environmental emissions, whereas a higher lignin content led to lower emissions, as shown in Section 3.3.2. The variation in lignin content was examined within a range of $\pm 20\%$. The lignin content in the biomass composition has a significant impact, as shown in Fig. 10. Increasing the initial lignin content leads to a decrease in environmental emissions, whereas a reduction in lignin content results in higher emissions, also due to interactions with other unit operations in the system, as discussed in Section 3.3.2.

Concerning the dynamic LCA, the most important parameters leading the uncertainty on the dynamic LCA results are the process occurrence time and the climate model uncertainty. IPCC models induce an uncertainty on iRF of $\pm 18\%$ to $\pm 26\%$ from 20 to 100 years. The uncertainty on GMTCC varies from $\pm 45\%$ to $\pm 90\%$ for 20 to 100 years (Myhre et al., 2014).

The most important time interval is from zero to 100 years (on Fig. 7), where the temporal carbon storage in biobased products can occur. Notably, the life time of those products will determine both the net values of iRF and GMTCC, and the duration of the potential cooling effect, as shown in Fig. 7 for a lifetime of 20 years and 40 years (values

representative for furniture, for instance). As the biobased product containing lignin is not specified, the analysis gives the variation intervals of the impact indicators (Fig. 7).

4. Conclusions

Environmental performance assessment of low-TRL technologies needs scaled-up data in order to build LCI. The development of a process flow diagram for a low-TRL organosolv process (AST) for lignin extraction using 1-butanol was successfully demonstrated, resulting in a robust and reliable inventory of mass and energy flows. Common data limitations were effectively addressed through a simulation-based methodology, enabling a comprehensive life cycle assessment that highlighted the environmental trade-offs associated with key process parameters. Simulation results in terms of energy consumption and yield were validated against literature. A simplified method was also applied to calculate the material and energy flows, based on chemical engineering rules, without using a simulation software.

The AST environmental performance is led by the trade-offs between the solvent use and heat necessary to its internal recycling, the two main contributors in 23 out of the 24 impact categories. The solvent type and origin, as well as the type of energy used are crucial for the environmental overall performance of the organosolv process.

The simplified method approximates the energy and water consumptions, and the impact results deviate from the rigorous simulation results in the range (-50% , $+63\%$). Simplified method does not adequately account for complex internal recycling, of solvent and water for instance, which is essential for making a technology competitive; however, it could be used for a preliminary evaluation.

The influence of future energy production routes was investigated through pLCA using premise tool. The slight reduction of climate change impact (GWP₁₀₀) by 2050, observed for AST with enhanced solvent recovery (AST-SR), is explained by the already low-carbon energy mix in France. Regardless of the scenario, the decrease in the climate change impact over time correlates with an increase in mineral/metal depletion (ADP) and human toxicity (minerals), due to the replacement of fossil fuels with nuclear and renewable energy production, which requires intensive use of minerals/metals.

Dynamic LCA approach highlighted the importance of considering the biogenic carbon capture and emissions with their dynamics, for the climate change impact evaluation. While static LCA considers no contribution of biogenic CO₂, and calculates an impact of 1.2 kg CO₂-eq, the dynamic approach clearly demonstrates the climate benefit of producing and utilizing lignin from wood. However, this benefit is limited in time and strongly depends on the end-of-life management. Incineration of the material should be avoided as it shifts the net result to warming effect.

Pearson analysis was applied to 9 process performance parameters

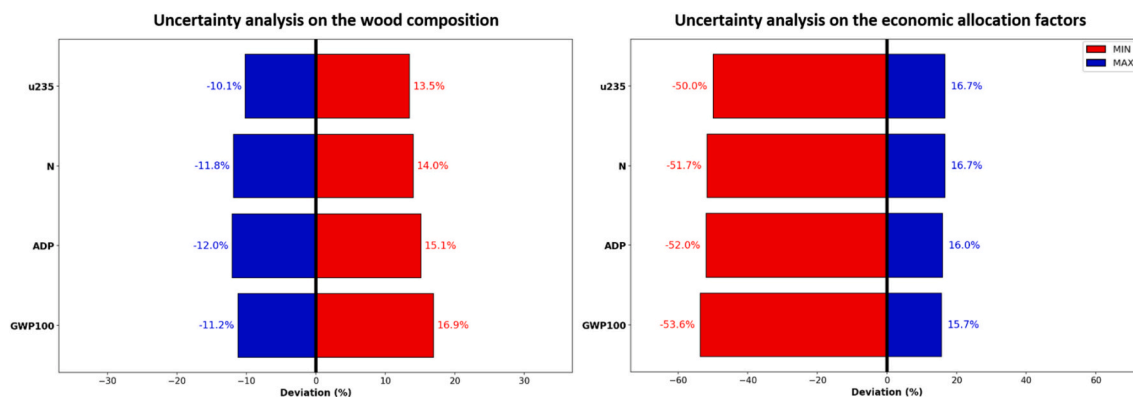


Fig. 10. Uncertainty Analysis of Economic Allocation Factors and Biomass Composition: Results for Ionising Radiation (U-235), Marine Eutrophication (N), Mineral Resource Depletion (ADP), and Climate change, global warming potential (GWP100) (all results are presented in Section 8.2 of the SI).

and 24 impact categories. Concerning the impact categories, the analysis showed strong interdependencies across all categories, supporting the selection of GWP₁₀₀ as a representative indicator. Supported by Principal Component Analysis, the set of performance indicators was reduced to four: lignin yield, water input, and total heat demand, and GWP₁₀₀. As expected, this later demonstrated strong negative correlation with lignin yield, strong positive correlation with heat demand, and weak positive correlation with water consumption. Parametric analysis, conducted on 20 process parameters, highlighted the strong sensitivity of the performances to the biomass composition, the conversion of lignin dissolution, the cake moisture achieved in filtration steps, and distillate flow rate (in distillation column for solvent recovery). The uncertainty analysis further confirmed these trends, identifying biomass composition and economic allocation factors as major contributors to variability in the results.

In this work, different and complementary methods were employed to uncover the potential technical and environmental performances of an emerging technology. The proposed methodology provides a flexible and transparent framework for generating consistent LCIs and environmental assessments, thereby supporting informed decision-making and scale-up at early development stages.

CRedit authorship contribution statement

Rafic El Kazzi: Writing – original draft, Visualization, Software, Investigation, Data curation. **Carlos Eduardo Robles-Rodriguez:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Ligia Tiruta-Barna:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Aras Ahmadi:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This work was supported by the European Union under the grant number 101135371 – project LCA4Bio.

Appendix A. Supplementary data

The supporting information document contains detailed description of methods and parameters used for process modeling and simulation. All LCA results are provided. Calculation flowsheets are available on request. Supplementary data to this article can be found online at <http://doi.org/10.1016/j.biteb.2026.102829>.

Data availability

Data will be made available on request.

References

- Abdelkafi, F., Ammar, H., Rousseau, B., Tessier, M., El Gharbi, R., Fradet, A., 2011. Structural analysis of alfa grass (*Stipa tenacissima* L.) lignin obtained by acetic acid/formic acid delignification. *Biomacromolecules* 12 (11), 3895–3902. <https://doi.org/10.1021/bm2008179>.
- Abdi, H., Williams, L.J., 2010. Principal component analysis. *WIREs Comput. Stat.* 2 (4), 433–459. <https://doi.org/10.1002/wics.101>.

- Aden, A., et al., 2002. Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover. NREL/TP-510-32438, 15001119. <https://doi.org/10.2172/15001119>.
- Ahmadi, A., et al., 2019. Eco-design approach for an innovative production process of low molar mass dextran. *Green Chem.* 21, 4512–4531. TBI, Université de Toulouse, CNRS, INRA, INSA, Toulouse, France, 135 Avenue de Rangueil, 31077, Toulouse, France.
- Ali, M., 2014. RFI Category 1 – LIGNOCELLULOSIC SUGARS. American Science and Technology Corporation.
- Alsosy Altinkaya, S., 2024. A perspective on cellulose dissolution with deep eutectic solvents. *Front. Membr. Sci. Technol.* 3. <https://doi.org/10.3389/frmst.2024.1382054>.
- Alvira, P., Tomás-Pejó, E., Ballesteros, M., Negro, M.J., 2010. Pretreatment technologies for an efficient bioethanol production process based on enzymatic hydrolysis: a review. *Bioresour. Technol.* 101 (13), 4851–4861. <https://doi.org/10.1016/j.biortech.2009.11.093>.
- Andreas, B.S., et al., 2023. Updated characterisation and normalisation factors for the Environmental Footprint 3.1 method. JRC Publications Repository. <https://publications.jrc.ec.europa.eu/repository/handle/JRC130796>. (Accessed 21 April 2026).
- Arvidsson, R., et al., 2018. Environmental assessment of emerging technologies: recommendations for prospective LCA. *J. Ind. Ecol.* 22 (6), 1286–1294. <https://doi.org/10.1111/jiec.12690>.
- Azad, T., Schuler, J.D., Auad, M.L., Elder, T., Adamczyk, A.J., 2020. Model lignin oligomer pyrolysis: coupled conformational and thermodynamic analysis of β-O-4' bond cleavage. *Energy Fuel* 34 (8), 9709–9724. <https://doi.org/10.1021/acs.energyfuels.0c01573>.
- Baumstark, L., et al., 2021. REMIND2.1: transformation and innovation dynamics of the energy-economic system within climate and sustainability limits. *Geosci. Model Dev.* 14 (10), 6571–6603. <https://doi.org/10.5194/gmd-14-6571-2021>.
- Brosse, N., Hussin, M.H., Rahim, A.A., 2019. Organosolv processes. In: Wagemann, K., Tippkötter, N. (Eds.), *Biorefineries*. Springer International Publishing, Cham, pp. 153–176. <https://doi.org/10.1007/978-3-319-61616-1>.
- Climate Change Impact Tool, 2024. INSA Toulouse. Accessed: Feb. 18, 2026. [Online]. Available: <https://www.insa-toulouse.fr/cii-tool/>.
- Cucurachi, S., Steubing, B., Siebler, F., Navarre, N., Caldeira, C., Sala, S., 2022. Prospective LCA methodology for Novel and Emerging Technologies for BIO-based products - The PLANET BIO project. In: JRC Publications Repository. Accessed: Apr. 09, 2026. [Online]. Available: <https://publications.jrc.ec.europa.eu/repository/handle/JRC129632>.
- Deckmyn, G., Muys, B., García Quijano, J., Ceulemans, R., 2004. Carbon sequestration following afforestation of agricultural soils: comparing oak/beech forest to short-rotation poplar coppice combining a process and a carbon accounting model. *Glob. Chang. Biol.* 10, 1482–1491. <https://doi.org/10.1111/j.1365-2486.2004.00832.x>.
- Ekvall, T., Finnveden, G., 2001. Allocation in ISO 14041—a critical review. *J. Clean. Prod.* 9 (3), 197–208. [https://doi.org/10.1016/S0959-6526\(00\)00052-4](https://doi.org/10.1016/S0959-6526(00)00052-4).
- Erakca, M., Baumann, M., Helbig, C., Weil, M., 2024. Systematic review of scale-up methods for prospective life cycle assessment of emerging technologies. *J. Clean. Prod.* 451, 142161. <https://doi.org/10.1016/j.jclepro.2024.142161>.
- Fabiola, 2024. TNO Ventures. Accessed: May 16, 2025. [Online]. Available: <https://ventures.tno.nl/portfolio/fabiola/>.
- González, M., Tejado, A., Peña, C., Labidi, J., 2008. Organosolv pulping process simulations. *Ind. Eng. Chem. Res.* 47 (6), 1903–1909. <https://doi.org/10.1021/ie070432j>.
- Groen, E., Heijungs, R., Bokkers, E.A.M., Boer, I.J.M., 2014. *Sensitivity Analysis in Life Cycle Assessment*.
- Herry, A., 2020. Large Scale Lignin Organosolv Extraction. bachelor. Accessed: Oct. 20, 2025. [Online]. Available: <https://fse.studenttheses.ub.rug.nl/22380/>.
- Ibbett, R., Gaddipati, S., Davies, S., Hill, S., Tucker, G., 2011. The mechanisms of hydrothermal deconstruction of lignocellulose: new insights from thermal–analytical and complementary studies. *Bioresour. Technol.* 102 (19), 9272–9278. <https://doi.org/10.1016/j.biortech.2011.06.044>.
- Intergovernmental Panel on Climate Change (IPCC), 2023. *Climate Change 2021 – The Physical Science Basis: Working Group I Contribution to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*. Cambridge University Press, Cambridge. <https://doi.org/10.1017/9781009157896>.
- ISO, 2006a. ISO 14040:2006. ISO. Accessed: Jun. 26, 2024. [Online]. Available: <https://www.iso.org/fr/standard/37456.html>.
- ISO, 2006b. ISO 14044:2006. ISO. Accessed: Jun. 26, 2024. [Online]. Available: <https://www.iso.org/fr/standard/38498.html>.
- Jolliffe, I.T., Cadima, J., 2016. Principal component analysis: a review and recent developments. *Philos. Trans. A Math Phys. Eng. Sci.* 374 (2065), 20150202. <https://doi.org/10.1098/rsta.2015.0202>.
- Kautto, J., Realff, M., Ragauskas, A., Kässi, T., 2014. Economic analysis of an organosolv process for bioethanol production. *BioResources* 9, 6041–6072. <https://doi.org/10.15376/biores.9.4.6041-6072>.
- Kimita, K., Brambila-Macias, S.A., Tillman, A.-M., Sakao, T., 2021. Failure analysis method for enhancing circularity through systems perspective. *J. Ind. Ecol.* 25 (3), 544–562. <https://doi.org/10.1111/jiec.13069>.
- Köchermann, J., Mühlenberg, J., Klemm, M., 2018. Kinetics of hydrothermal furfural production from organosolv hemicellulose and D-xylose. *Ind. Eng. Chem. Res.* 57, 14417–14427. <https://doi.org/10.1021/acs.iecr.8b03402>.
- Kravanja, P., Modarresi, A., Friedl, A., 2013. Heat integration of biochemical ethanol production from straw – a case study. *Appl. Energy* 102, 32–43. <https://doi.org/10.1016/j.apenergy.2012.08.014>.

- Lange, H., Decina, S., Crestini, C., 2013. Oxidative upgrade of lignin – recent routes reviewed. *Eur. Polym. J.* 49 (6), 1151–1173. <https://doi.org/10.1016/j.eurpolymj.2013.03.002>.
- Learn Brightway' Book — Learn Brightway, 2024. Accessed: Jun. 02, 2025. [Online]. Available: <https://learn.brightway.dev/en/latest/content/home.html>.
- Li, W., et al., 2018. Fractionation and characterization of lignin streams from unique high-lignin content endocarp feedstocks. *Biotechnol. Biofuels* 11. <https://doi.org/10.1186/s13068-018-1305-7>.
- Lora, J.H., Glasser, W.G., 2002. Recent industrial applications of lignin: a sustainable alternative to nonrenewable materials. *J. Polym. Environ.* 10 (1), 39–48. <https://doi.org/10.1023/A:1021070006895>.
- Manesh, A., 2014. RFI Category 2 – LIGNIN. American Science and Technology Corporation.
- Manesh, A., Hemyeri, R., Mohapatra, S., Guenther, J., Zoborowski, E., 2014. System and Method for Extractions of Chemicals from Lignocellulosic Materials. American Science and Technology Corporation.
- Market for electricity, medium voltage. In: France - electricity, medium voltage, 2024. ecoQuery. Accessed: Jan. 29, 2026. [Online]. Available: <https://ecoquery.ecoinvent.org/3.11/cutoff/dataset/6600/exchanges>.
- Méndez Seviliano, D., Wielen, L., Hooshyar, N., Ottens, M., 2014. MPP-UNIFAC, a predictive activity coefficient model for polyphenols. *Fluid Phase Equilibria* 384, 82–88. <https://doi.org/10.1016/j.fluid.2014.10.020>.
- Mesa, L., López, N., Cara, C., Castro, E., González, E., Mussatto, S.I., 2016. Techno-economic evaluation of strategies based on two steps organosolv pretreatment and enzymatic hydrolysis of sugarcane bagasse for ethanol production. *Renew. Energy* 86, 270–279. <https://doi.org/10.1016/j.renene.2015.07.105>.
- Mishra, S., et al., 2017. Principal component analysis. *Int. J. Livest. Res.* 1. <https://doi.org/10.5455/ijlr.20170415115235>.
- Moncada, J., Vural Gursel, I., Huijgen, W.J.J., Dijkstra, J.W., Ramírez, A., 2018. Techno-economic and ex-ante environmental assessment of C6 sugars production from spruce and corn. Comparison of organosolv and wet milling technologies. *J. Clean. Prod.* 170, 610–624. <https://doi.org/10.1016/j.jclepro.2017.09.195>.
- Mörck, R., Reimann, A., Kringstad, K.P., 1988. Fractionation of Kraft lignin by successive extraction with organic solvents. III. Fractionation of Kraft lignin from birch. *Holzforschung* 111–116. <https://doi.org/10.1515/hfsg.1988.42.2.111>.
- Moretti, C., et al., 2020a. Reviewing ISO compliant multifunctionality practices in environmental life cycle modeling. *Energies* 13 (14), 3579. <https://doi.org/10.3390/en13143579>.
- Moretti, C., et al., 2020b. Combining biomass gasification and solid oxid fuel cell for heat and power generation: an early-stage life cycle assessment. *Energies* 13 (11), 2773. <https://doi.org/10.3390/en13112773>.
- Moretti, C., Corona, B., Hoefnagels, R., Vural-Gürsel, I., Gosselink, R., Junginger, M., 2021. Review of life cycle assessments of lignin and derived products: lessons learned. *Sci. Total Environ.* 770, 144656. <https://doi.org/10.1016/j.scitotenv.2020.144656>.
- Mukherjee, A., Mandal, T., Ganguly, A., G., P.S., Chatterjee, P.K., 2017. Investigations on the kinetics of acid catalyzed hemicellulose hydrolysis derived from waste rice straw for the production of bio-ethanol. *INDJST* 10 (11), 1–8. <https://doi.org/10.17485/ijst/2017/v10i11/92605>.
- Myhre, G., et al., 2014. Anthropogenic and Natural Radiative Forcing. <https://doi.org/10.1017/CBO9781107415324.018>.
- Nickel, L., 2022. Product Environmental Footprint (PEF) - A Complete Overview. Ecochain LCA Software. Accessed: May 15, 2025. [Online]. Available: <https://ecochain.com/blog/product-environmental-footprint/>.
- Nitzsche, R., Budzinski, M., Gröngröft, A., 2016. Techno-economic assessment of a wood-based biorefinery concept for the production of polymer-grade ethylene, organosolv lignin and fuel. *Bioresour. Technol.* 200, 928–939. <https://doi.org/10.1016/j.biortech.2015.11.008>.
- Nurdiawati, A., Mir, B.A., Al-Ghamdi, S.G., 2025. Recent advancements in prospective life cycle assessment: current practices, trends, and implications for future research. *Resour. Environ. Sustain.* 20, 100203. <https://doi.org/10.1016/j.resenv.2025.100203>.
- Nyman, E., 2026. European Pulp Prices: The Impact of Supply and Demand. Fastmarkets. Accessed: Apr. 22, 2026. [Online]. Available: <https://www.fastmarkets.com/insights/european-pulp-prices-climb-amid-ongoing-bek-and-nbsk-negotiations/>.
- Patel, A.D., Meesters, K., Den Uil, H., De Jong, E., Blok, K., Patel, M.K., 2012. Sustainability assessment of novel chemical processes at early stage: application to biobased processes. *Energ. Environ. Sci.* 5 (9), 8430. <https://doi.org/10.1039/c2ee21581k>.
- Peres, A.M., Macedo, E.A., 1997. A modified UNIFAC model for the calculation of thermodynamic properties of aqueous and non-aqueous solutions containing sugars. *Fluid Phase Equilib.* 139 (1), 47–74. [https://doi.org/10.1016/S0378-3812\(97\)00196-9](https://doi.org/10.1016/S0378-3812(97)00196-9).
- Piccinno, F., Hirschier, R., Seeger, S., Som, C., 2016. From laboratory to industrial scale: a scale-up assessment for chemical processes in life cycle assessment studies. *J. Clean. Prod.* 135. <https://doi.org/10.1016/j.jclepro.2016.06.164>.
- Prasad, A., Sotenko, M., Blenkinsopp, T., Coles, S.R., 2016. Life cycle assessment of lignocellulosic biomass pretreatment methods in biofuel production. *Int. J. Life Cycle Assess.* 21 (1), 44–50. <https://doi.org/10.1007/s11367-015-0985-5>.
- Prausnitz, J.M., Lichtenthaler, R.N., de Azevedo, E.G., 1998. *Molecular Thermodynamics of Fluid-Phase Equilibria*. Pearson Education.
- Rameshkumar, S., Panjiyan, K., Danaee, I., M, O., 2022. A New Method for Determination of Molecular Weight of Compounds Soluble in Protic Solvents by Electrochemical Impedance Spectroscopy. <https://doi.org/10.5772/intechopen.106558>.
- Reith, J.H., Huijgen, W.J.J., van de Laan, R.R., 2008. Modified organosolv as a fractionation process of lignocellulosic biomass for co-production of fuels and chemicals. Accessed: Oct. 20, 2025. [Online]. Available: <https://resolver.tno.nl/uu/id:3aa14fa0-e875-410e-9b36-221b8c00e33c>.
- Rinaldi, R., et al., 2016. Paving the way for lignin valorisation: recent advances in bioengineering, biorefining and catalysis. *Angew. Chem. Int. Ed.* 55 (29), 8164–8215. <https://doi.org/10.1002/anie.201510351>.
- Romina, C., Antonio, B., Alessandra, T., Giuseppina, A., 2025. A framework for LCA analysis of low TRL products: towards a sustainable approach in early development stages. *Proc. Comput. Sci.* 253, 3151–3159. <https://doi.org/10.1016/j.procs.2025.02.040>.
- Ryan, N., Yaseneva, P., 2021. A critical review of life cycle assessment studies of woody biomass conversion to sugars. *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.* 379 (2206), 20200335. <https://doi.org/10.1098/rsta.2020.0335>.
- Sacchi, R., et al., 2022. Prospective Environmental Impact asSement (premise): a streamlined approach to producing databases for prospective life cycle assessment using integrated assessment models. *Renew. Sustain. Energy Rev.* 160, 112311. <https://doi.org/10.1016/j.rser.2022.112311>.
- Saltelli, A. (Ed.), 2008. *Global Sensitivity Analysis: The Primer*. John Wiley, Chichester, England Hoboken, NJ. <https://doi.org/10.1002/9780470725184>.
- Schober, P., Boer, C., Schwarte, L.A., 2018. Correlation coefficients: appropriate use and interpretation. *Anesth. Analg.* 126 (5), 1763–1768. <https://doi.org/10.1213/ANE.0000000000002864>.
- Scopus preview, 2026. Scopus - Welcome to Scopus. Accessed: Oct. 28, 2025. [Online]. Available: <https://www.scopus.com/home.uri?zone=header&origin=browse>.
- Seader, J.D., Henley, E.J., Roper, D.K., 2010. *Separation Process Principles*, 3rd edition. John Wiley Incorporated.
- Segers, B., et al., 2024. Lignocellulosic biomass valorisation: a review of feedstocks, processes and potential value chains and their implications for the decision-making process. *RSC Sustain.* 2 (12), 3730–3749. <https://doi.org/10.1039/D4SU00342J>.
- Sheikholeslami, Z., Ehteshami, M., Nazif, S., Semiaran, A., 2023. The uncertainty analysis of life cycle assessment for water and wastewater systems: review of literature. *Alex. Eng. J.* 73, 131–143. <https://doi.org/10.1016/j.aej.2023.04.039>.
- Simon, B., Bachtin, K., Kilic, A., Amor, B., Weil, M., 2016. Proposal of a Framework for Scale-Up Life Cycle Inventory: A Case of Nanofibers for Lithium Iron Phosphate Cathode Applications. *Jun.* 09.
- Smit, A.T., Verges, M., Schulze, P., van Zomeren, A., Lorenz, H., 2022. Laboratory- to pilot-scale fractionation of lignocellulosic biomass using an acetone organosolv process. *ACS Sustain. Chem. Eng.* 10 (32), 10503–10513. <https://doi.org/10.1021/acscuschemeng.2c01425>.
- Tirutu-Barna, L., 2021. A climate goal-based, multicriteria method for system evaluation in life cycle assessment. *Int. J. Life Cycle Assess.* 26. <https://doi.org/10.1007/s11367-021-01991-1>.
- Tirutu-Barna, L., 2026. Expanding the dynamic climate change impact model for dynamic LCA based on the climate science. *Int. J. Life Cycle Assess.* 31 (1), 27. <https://doi.org/10.1007/s11367-026-02583-7>.
- Tofani, G., Jasiukaitytė, E., Grilc, M., Likozar, B., 2023. Organosolv biorefinery: Resource-based process optimisation, pilot technology scale-up and economics. *Green Chem.* <https://doi.org/10.1039/D3GC03274D>.
- Trubetskaya, A., et al., 2016. Comparison of high temperature chars of wheat straw and rice husk with respect to chemistry, morphology and reactivity. *Biomass Bioenergy* 86, 76–87. <https://doi.org/10.1016/j.biombioe.2016.01.017>.
- Tuomisto, H.L., Allan, S.J., Ellis, M.J., 2022. Prospective life cycle assessment of a bioprocess design for cultured meat production in hollow fiber bioreactors. *Sci. Total Environ.* 851, 158051. <https://doi.org/10.1016/j.scitotenv.2022.158051>.
- U.S. Environmental Protection Agency - GWPs, 2023. Data.gov. Accessed: Apr. 21, 2026. [Online]. Available: <http://catalog.data.gov/dataset/ipcc-ar4-ar5-and-ar6-20-100-and-500-year-gwps>.
- User Guide, 2025. Premise 2.2.0 Documentation. Accessed: Jan. 30, 2026. [Online]. Available: <https://premise.readthedocs.io/en/latest/>.
- Viell, J., Harwardt, A., Seiler, J., Marquardt, W., 2013. Is biomass fractionation by Organosolv-like processes economically viable? A conceptual design study. *Bioresour. Technol.* 150, 89–97. <https://doi.org/10.1016/j.biortech.2013.09.078>.
- Wang, T.-P., et al., 2021. Structures and pyrolytic characteristics of organosolv lignins from typical softwood, hardwood and herbaceous biomass. *Ind. Crops Prod.* 171, 113912. <https://doi.org/10.1016/j.indcrop.2021.113912>.
- Watkins, K., Fatehi, P., 2026. A review on lignin extraction processes at different production scales. *Ind. Crops Products* 239, 122526. <https://doi.org/10.1016/j.indcrop.2025.122526>.
- Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., Weidema, B., 2016. The ecoinvent database version 3 (part I): overview and methodology. *Int. J. Life Cycle Assess.* 21 (9), 1218–1230. <https://doi.org/10.1007/s11367-016-1087-8>.
- What are IAMs? – IAMC. Accessed: Jan. 28, 2026. [Online]. Available: <https://www.iamconsortium.org/what-are-iams/>.
- Wood Pulp IndexMundi. In: Wood Pulp - Monthly Price (Euro per Metric Ton) - Commodity Prices - Price Charts, Data, and News - IndexMundi, 2026. Accessed: Apr. 22, 2026. [Online]. Available: <https://www.indexmundi.com/commodities/?commodity=wood-pulp&months=120¤cy=eur>.
- Zeilerbauer, L., Lindorfer, J., Süß, R., Kamm, B., 2021. Techno-economic and life-cycle assessment of a wood chips-based organosolv biorefinery concept for production of lignin monomers and oligomers by base-catalyzed depolymerization. *Biofuels Bioprod. Biorefin.* 16, 370–388. <https://doi.org/10.1002/bbb.2315>.
- Zhao, X., Cheng, K., Liu, D., 2009. Organosolv pretreatment of lignocellulosic biomass for enzymatic hydrolysis. *Appl. Microbiol. Biotechnol.* 82, 815–827. <https://doi.org/10.1007/s00253-009-1883-1>.