

Economic and Environmental Evaluation of Sequential vs Single-Reactor Tandem Catalytic Routes for Furan-Derived Amine Production

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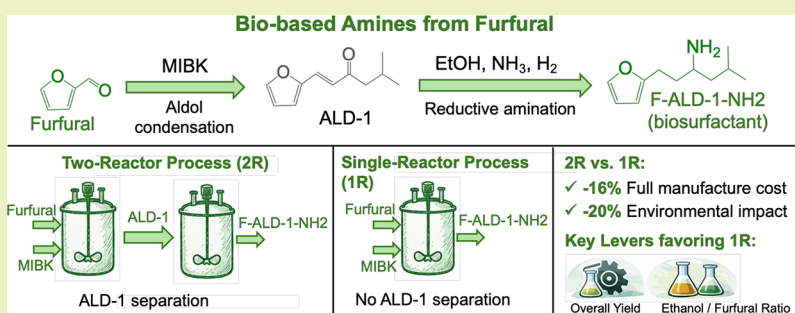
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ABSTRACT: The development of intensified catalytic processes for biomass valorization is a key strategy to improve the sustainability of chemical manufacturing. In this work, we compare a conventional two-reactor and a single-reactor tandem process for the production of the furfural-derived amine 1-(furan-2-yl)-4-methylpentan-2-amine (F-ALD-1-NH₂), combining technoeconomic analysis (TEA) and cradle-to-gate life cycle assessment (LCA). Both routes involve aldol condensation of furfural with methyl isobutyl ketone followed by reductive amination but differ in process configuration, yields, and catalyst requirements. Under base-case conditions, the two-reactor process outperforms the single-reactor configuration, exhibiting 16–20% lower full manufacturing cost (€5250/ton vs €6313/ton) and systematically reduced environmental impacts across all midpoint categories (e.g., 21% lower global warming potential). These differences are primarily driven by the higher overall yield (91% vs 74%) and lower catalyst loading of the two-reactor process. However, sensitivity analysis reveals that process intensification becomes advantageous under optimized conditions. By improving yield, reducing catalyst loading, and optimizing solvent ratios, the single-reactor process could achieve up to 10% lower manufacturing cost and 5–20% lower environmental impacts relative to the two-reactor configuration. Across both routes, key drivers of cost and environmental performance include furfural and solvent consumption, catalyst loading and regeneration, and energy demand for separations. Uncertainty analysis confirms the statistical robustness of these trends for selected impact categories. This study demonstrates that while process intensification does not inherently guarantee improved sustainability, it can deliver significant economic and environmental benefits when reaction performance and process parameters are carefully optimized. These findings highlight the importance of integrating early-stage TEA and LCA to guide the design and development of intensified catalytic processes for renewable chemical production.

KEYWORDS: furfural, ruthenium, amination, life cycle assessment, technoeconomic analysis

1. INTRODUCTION

The transition toward more sustainable chemical manufacturing requires not only the replacement of fossil-based feedstocks with renewable alternatives but also the development of more efficient processes.^{1–3} Process intensification has emerged as a key strategy, aiming to reduce process complexity, energy demand, and material consumption while maintaining or enhancing product performance.^{1–4} In particular, intensified catalytic processes that integrate multiple transformations within a single reactor offer promising opportunities to improve both economic and environmental performance.^{2–4}

Biomass-derived platform molecules play a central role in enabling such strategies.^{5–7} Among them, furfural (FF) stands out due to its large-scale availability from lignocellulosic residues and its versatility as a chemical intermediate.^{7,8} As one of

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the top value-added chemicals derived from biomass, FF is produced at an industrial scale (>200 kt year $^{-1}$) and remains relatively inexpensive (€1.0–1.2/kg),⁹ making it an attractive feedstock for the synthesis of fuels, solvents, and functionalized chemicals.^{6,7,10,11} In particular, nitrogen-containing compounds derived from FF are of growing interest, as amines constitute key intermediates in pharmaceuticals, agrochemicals, and advanced materials.¹² However, their current production largely relies on fossil-based resources and multistep synthetic pathways, highlighting the need for more sustainable alternatives.

Catalytic methodologies enabling the direct conversion of renewable substrates into amines represent an important research direction. Reductive amination of biomass-derived aldehydes and ketones has attracted increasing attention, especially when implemented using heterogeneous catalysts that facilitate catalyst recovery and process scalability.^{13–17} In this context, the aldol condensation of FF with ketones, followed by subsequent upgrading steps, has been widely explored as a route to tailor carbon chain length and functionality.¹⁸ Such transformations can be carried out either in sequential reactors or in a single reactor using multifunctional or bifunctional catalytic systems.^{19–28} Compared to conventional multistep configurations, single-reactor configurations offer clear advantages in terms of process intensification, notably by eliminating intermediate separation steps and reducing solvent use.

Recent advances in catalysis have further expanded these possibilities. In particular, a ruthenium-based catalytic system has been reported for the direct transformation of FF into furan-derived amines, enabling tandem aldol condensation and reductive amination in a single process.²⁹ This chemistry can be implemented either as a conventional two-step route or as a one-pot tandem process, providing a relevant case study to assess the benefits and limitations of process intensification. While single-reactor configurations are often assumed to be inherently more sustainable, their actual performance depends on multiple factors, including catalytic efficiency, selectivity, operating conditions, and downstream processing requirements. Trade-offs may arise, for instance, from reduced yields, increased byproduct formation, or higher sensitivity to process parameters. Consequently, quantitative evaluation using combined technoeconomic and environmental metrics is essential to determine whether process intensification leads to tangible benefits.

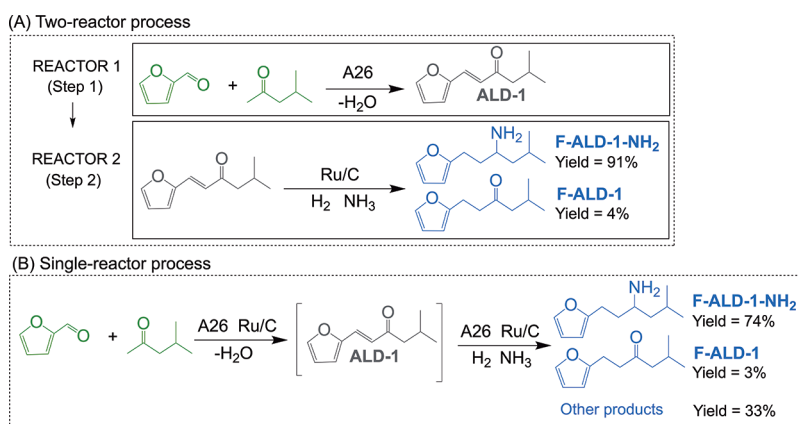
In this work, we performed a combined technoeconomic analysis (TEA) and life cycle assessment (LCA) to compare a two-reactor and a single-reactor tandem route for the production of 1-(furan-2-yl)-4-methylpentan-2-amine (F-ALD-1-NH₂), a potential biosurfactant derived from FF. The process involves (i) aldol condensation–crotonization of FF with methyl isobutyl ketone (MIBK) to form (*E*)-1-(furan-2-yl)-5-methylhex-1-en-3-one (ALD-1), followed by (ii) reductive amination to yield F-ALD-1-NH₂ (Scheme 1A). Both configurations differ in process integration, catalyst requirements, and product distribution, with comparable conversions (95%) but distinct overall yields (74% vs 91%) and byproduct formation, including ring-opening pathways in the single-reactor system (Scheme 1B; see ref 29 for experimental details and the Supporting Information). In the former case, ring-opening byproducts are generated covering 18% of carbon loss.

By estimating the full manufacturing cost (FMC) and quantifying environmental impacts at the cradle-to-gate level, this study aims to identify the key drivers governing process performance and to determine under which conditions process intensification becomes advantageous. More broadly, this work highlights the importance of integrating TEA and LCA at early stages of process development to guide the design and selection of intensified catalytic routes for sustainable biomass valorization.^{30,31}

TEA and LCA have been widely proven effective for evaluating emerging technologies at early stages of development, enabling researchers to identify economic and environmental hotspots and guide R&D priorities. At the current laboratory-scale stage, detailed process design is not warranted given the uncertainties in reaction performance, catalyst stability, and scale-up behavior. The objective is to identify key drivers and compare process configurations under consistent assumptions, not to produce a definitive plant design. A comprehensive sensitivity analysis tests the robustness of conclusions against variations in key assumptions.

This study builds on our previous work on the production of 5-methyl-1-(tetrahydrofuran-2-yl)hexan-3-one (THF-ALD-1) as a biosolvent, where process intensification in a single reactor demonstrated both economic and environmental benefits compared to a two-reactor configuration.³² In that case, cost

Scheme 1. (A) Two-Reactor and (B) Single-Reactor Tandem Processes to Produce the F-ALD-1-NH₂ Biosurfactant *via* the Reaction of FF with MIBK Followed by Reductive Amination with NH₃ and H₂ with Byproducts 1-(Furan-2-yl)-5-methylhexan-3-one (F-ALD-1) and Ring-Opening Products (Other Products)^a



^aThe experimental protocols for both synthetic routes are listed in the Supporting Information.²⁹

reductions of up to 11% and significant decreases across multiple environmental impact categories (terrestrial ecotoxicity potential, photochemical oxidant creation potential, and acidification potential) were achieved. The present study extends this approach to nitrogen-containing compounds, providing new insights into the interplay between catalytic performance, process design, and sustainability metrics in intensified reactors.

2. TECHNOECONOMIC ANALYSIS AND LIFE CYCLE ASSESSMENT

2.1. Methodological Framework

This study combines technoeconomic analysis (TEA) and life cycle assessment (LCA) following a five-step framework aligned with ISO 14040:2006 and ISO 14044:2006:³³ (i) goal and scope definition, (ii) life cycle inventory (LCI) compilation, (iii) life cycle impact assessment (LCIA), (iv) cost evaluation, and (v) interpretation of results. All inventory modeling and impact assessments were performed using SimaPro 9.1 with the Ecoinvent 3.4 database. Emission factors used for estimating the transport contribution to base-case calculations were obtained from the Ecoinvent v3.8 database. Unit costs for raw materials and process inputs are summarized in Table 1.

2.2. Goal, Scope, and System Definition

2.2.1. Goal and Functional Unit. The objective of this work is to perform a cradle-to-gate LCA for F-ALD-1-NH₂ production, comparing single-reactor and two-reactor configurations. The functional unit was defined as 1 kg of F-ALD-1-NH₂ at the plant gate. The system boundaries comprised all upstream inputs required for production, including raw materials, solvents, catalysts, and utilities, up to the production gate

(excluding packaging and distribution). Transportation of reagents (e.g., FF, MIBK, and catalysts) was excluded from the base-case system boundary following preliminary screening, which indicated that transport contributes <3% to GWP and <8% to AP and POCP. A sensitivity case including realistic logistics scenarios for FF (ocean freight from China to Europe plus trucking) and all other raw materials (European trucking) confirmed that the comparative ranking of the two processes is unaffected. Full transport inventory data are provided in Table S1 with logistics assumptions and emission factors in Table S2 and Table S3, respectively.

2.2.2. Allocation Rules. Economic allocation was applied to ruthenium (Ru) based on average market prices over the past decade.³⁸ For FF, maize-derived feedstocks (grains, corn cob, and stover) were considered due to their predominance in current production routes. No allocation was applied between F-ALD-1-NH₂ and byproducts. This consistent methodological framework enables direct comparison of full manufacturing costs (FMC), identification of key economic and environmental drivers, and evaluation of process intensification benefits across both configurations.

2.3. Life Cycle Inventory (LCI)

2.3.1. Process Description. Two production routes were evaluated:

1. Single-reactor process: sequential aldol condensation-crotonization and reductive amination carried out in a single reactor without intermediate purification.
2. Two-reactor process: sequential reactions performed in separate reactors with intermediate purification.

Table 1. Primary Variables in Single-Reactor and Two-Reactor Processes

	variables	base case ^a	refs. ^d
Economics	FF, €/ton	1300	(a)
	MIBK, €/ton	1250	(b)
	NH ₃ , €/ton	2000	(c)
	H ₂ , €/ton	2000	(c)
	Ethanol 95%, €/ton	1000	(d)
	A26, €/ton	9000	(e)
	Ru/C, €/kg (fresh)	350,000	(f)
	Ru/C, €/ton (regenerated)	20,000	
	FF conversion, %	100/95	(g)
	FF → ALD-1 selectivity, %	100/100	(g)
	ALD-1 conversion, %	100/100	(g)
	ALD-1 → F-ALD-1-NH ₂ selectivity, % ^c	74/96	(g)
	Overall F-ALD-1-NH ₂ yield, %	74/91	(g)
LCA + Economics	A26 loading, wt %	−/5	(h)
	Ru/C loading, wt %	5/5	(h)
	NH ₃ consumption, % ^b	+10/+10	(h)
	H ₂ consumption, % ^b	+10/+10	(h)
	MIBK recycling rate, %	98/98	(h)
	Ethanol recycling rate, %	95/95	(h)
	Ru/C loss after each batch, %	0.05/0.05	(h)
	Ru/C regeneration/recycling, %	90/90	(h)
	Aqueous/organic waste	Yes	(i)
	Landfill	Yes	

^aIn LCA + Economics, values correspond to single-reactor/two-reactor processes. The “Base case” refers to the values used in the process inventory (Table S1). ^bExcess H₂ over the stoichiometric requirement. ^cF-ALD-1-NH₂ purification yield of 98%. ^dRefs.: (a) Business Analyst, Q4 2018 (ref 34); (b) Business Analyst, Q4 2018 (ref 35); (c) price for green H₂ (ref 36); (d) from Zibo Anquan Chemical Co., Ltd. (China) (ref 37); (e) based on internal Solvay (Syensqo) data; (f) Johnson Matthey Ru prices, Q2 2018 (ref 38); (g) data from ref 29 (lab-scale optimized reaction conditions); (h) process assumption; (i) “Yes”: on-site valorization of organic wastes by combustion in a boiler for steam generation (steam credit); “No”: wastes burned outside.

Throughout this work, “reaction yield” refers to the yield of an individual reaction step, whereas “overall yield” denotes the cumulative yield from FF to purified F-ALD-1-NH₂, excluding purification steps. The term “optimized scenario” refers to the hypothetical process conditions combining the improved overall yield, reduced catalyst loading, and optimized solvent ratios evaluated during the sensitivity analysis.

2.3.2. Inventory Development and Scaling. Inventory data were derived from primary laboratory experiments,²⁹ ensuring high-quality data. No secondary literature data were used for the core foreground system. Experimental data were scaled to industrial conditions by preserving mass and energy balances and applying standard process engineering scaling assumptions. The production capacity was set to 3300 tons/year with 8000 h/year operation, corresponding to a mid-scale specialty chemical process. While the scale-up involves inherent uncertainties, the comprehensive sensitivity analysis described in Section 3 was designed to test the robustness of the conclusions against variations in key assumptions.

Key parameters influencing economic and environmental performance are listed in Table 1, with physical and operational data provided in Table S4, S5 and S6, respectively. Process flow-sheets and Sankey diagrams are provided in Scheme 2 and Figures S1, S2. The specific scale-up factors, reactor sizing methodology, heat integration assumptions, separation efficiencies, and equipment performance correlations are detailed in Table S7. The scale-up methodology included: (i) reactor sizing based on residence time requirements derived from laboratory kinetics, assuming perfectly stirred mixture behavior with a 1.2× safety factor, and pressure vessel sizing following ASME Section VIII Division 1 standards; (ii) separation unit design, where distillation column requirements (MIBK recovery, ethanol recovery, and product purification) were estimated based on vapor–liquid equilibrium considerations, with heat duties

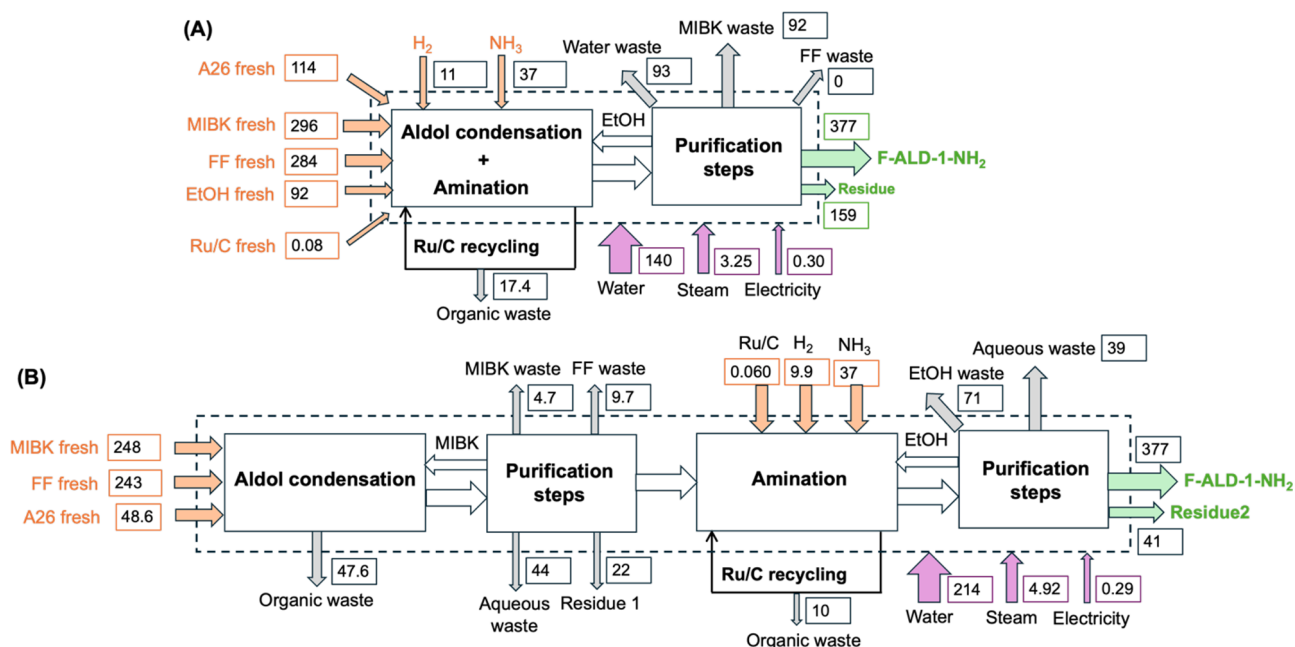
calculated for reboilers and condensers; (iii) heat integration through simplified pinch analysis to identify heat recovery opportunities between reactor effluents and feed preheating, with a 20% heat recovery efficiency assumed for the base case; and (iv) equipment costing using Taylor’s process step scoring method.

The scale-up from laboratory batch experiments to the industrial continuous process (3300 tons/year) inevitably involves uncertainties regarding reactor performance, heat integration efficiency, and separation yields. While mass and energy balances were preserved during scaling and standard process engineering correlations were employed (see Table S7 for a detailed breakdown of scale-up parameters), the assumed industrial performance—particularly in terms of product yield, catalyst productivity, and distillation efficiency—may not be fully realized in practice.

Importantly, the “best-case” scenario (100% overall yield, 5 wt % A26 loading) presented in this study represents a theoretical optimization target, not an experimentally validated condition. This scenario is included to illustrate the potential of process intensification under idealized conditions and to identify catalyst development priorities. Its industrial realization depends on continued catalyst development, stability validation, and pilot-scale demonstration.

The sensitivity analysis systematically evaluated the influence of key parameters, including overall yield, catalyst loading, solvent ratios, and regeneration frequency, on the economic and environmental outcomes. The results demonstrate that the comparative ranking between the single-reactor and two-reactor configurations remains robust across a wide range of parameter variations, with the two-reactor process consistently favored under base-case conditions and the single-reactor process only becoming advantageous when yield and catalyst loading are substantially optimized. The sensitivity analysis thus

Scheme 2. Simplified Flowsheet for (A) Single-Reactor and (B) Two-Reactor Processes^a



^aThe numbers refer to mass flows expressed in kg/h. Calculations for an F-ALD-1-NH₂ production line operational for 8000 h per year with an annual capacity of 3300 tons.

provides a transparent assessment of the uncertainties inherent in the scale-up and confirms that the main conclusions are not contingent on a single set of scale-up assumptions.

2.3.3. Background System Modeling. The background system was modeled using the Ecoinvent cutoff modeling approach. Global datasets (GLO) were preferentially used; European datasets (RER) were used when global data were unavailable.

Key energy-related datasets were harmonized across all inventories to ensure comparability. Steam demand was modeled using a European industrial natural-gas boiler (Heat, district or industrial, natural gas {Europe without Switzerland}|heat production, natural gas, at boiler condensing modulating >100 kW|Cutoff, U), representative of generic chemical-industry steam production. Electricity consumption was modeled using a European medium-voltage market mix (Electricity, medium voltage {RER}|market|Cutoff, U). Feedstock- and catalyst-related datasets include (Table S8) maize (GLO) and ruthenium (GLO) (Ecoinvent v3.4); MIBK (RER), electricity (RER), steam/heat (Europe w/o Switzerland), process water (RER), and H₂ (GLO) (Ecoinvent v3.6). Feedstock and catalyst datasets include maize and ruthenium (GLO) and MIBK, electricity, steam, process water, and hydrogen (RER/GLO), as detailed in Table S8.

2.3.4. Catalyst Manufacture and Recycling. We estimated the cost and environmental impact of 5 wt % Ru/C catalyst production. Environmental burdens for platinum group metal (PGM) production were allocated using a combination of mass-based (ore) and revenue (economic) methods including mining, beneficiation, metallurgy, separation, and refining.^{39,40} Economic allocation was adopted with periodic reassessment (Figures S3 and S4).

The Ru LCI was updated using 2010–2019 market data (superseding the older 1993–2002 data in Ecoinvent 3.4, {GLO}|market for update 2019|Cutoff, U), including primary (70%) and secondary (30%) sources.⁴¹ Primary production from South Africa and Russia was modeled separately and combined using market-weighted averages. The concentrations of Ru in the ore were assumed to be 0.44 and 0.3 ppm for South African and Russian ores, respectively.⁴² Table S8 lists the revised environmental impacts for Ru. The following LCI were created: Ruthenium {GLO}|market|Cutoff, U, Ruthenium {RU}|PGM mine operation|Cutoff, U, and Ruthenium {ZA}|PGM mine operation|Cutoff, U.

Catalyst regeneration was modeled assuming 90% Ru recovery efficiency. This value is a conservative estimate supported by recent literature on PGM and Ru recovery from spent catalysts. Hydrometallurgical leaching tests have demonstrated up to 100% Ru recovery in the volatilization step and 82% in conventional leaching,⁴³ while microwave-assisted leaching has achieved >90% recovery of Ru at temperatures above 150 °C. Industrial ruthenium recycling via distillation methods can achieve 85–99% recovery,⁴⁴ and mild regeneration methods have been shown to fully restore Ru/C catalyst activity. The dissolution of Ru is acknowledged to be more challenging than Pt or Pd due to the formation of a passivating RuO₂ layer,⁴³ supporting the use of a conservative 90% value. Catalyst losses and recycling costs (20,000 €/ton Ru) were included in both economic and environmental calculations. The required amount of fresh Ru as a function of the regeneration cycles (C) is presented in Table S9 and was used in the sensitivity analysis. Tables S10 and S11 provide the mass and energy balance per kg of Ru/C catalyst per regeneration cycle.

2.3.5. Biobased FF Production. Corncob-derived FF was selected as the representative biomass feedstock. The production process was based on an industrial-scale plant in Henan, China (600 ktons/year), including hydrolysis, dehydration, and steam stripping steps. The corresponding LCI was adapted from a previous study.³² This production location is representative of the current global FF supply (>80% of production). For the transport sensitivity case, we assumed ocean freight from Shanghai to Rotterdam (12,000 km) followed by trucking to the production site (500 km). While this increases the GWP by ~2% and AP/POCP by ~7–8%, the comparative conclusions remain unchanged. This scenario represents a conservative estimate, as actual FF shipments may be shorter (e.g., to Asian production sites) or longer (e.g., to Americas), but the sensitivity analysis confirms that the overall trends are not transport-dependent.

2.4. Life Cycle Impact Assessment (LCIA) Methods

2.4.1. Midpoint Impact Categories. Environmental impacts were quantified using 10 midpoint indicators from the CML 2001 method:⁴⁵ (1) climate change [GWP 100a], (2) primary energy demand (renewable [RE] and nonrenewable [NRE]), (3) ecotoxicity potential (human [HTP], freshwater ecotoxicity [FAETP], marine ecotoxicity [MAETP], and terrestrial ecotoxicity [TETP]), (4) water consumption [Water], (5) abiotic depletion potential [ADP], (6) quantitative land use [Land Use], (7) acidification potential [AP], (8) eutrophication potential [EP], (9) ozone layer depletion potential [OLDP], and (10) photochemical oxidant creation potential [POCP]. Biogenic CO₂ sequestration was included in GWP calculations. Definitions and units are provided in the Supporting Information (SI).

2.4.2. Impact Score Breakdown. Impacts were disaggregated by contributions from major process elements: (1) H₂, (2) NH₃, (3) waste treatment (incineration of organic waste), (4) heat (energy used for reactor and distillation columns), (5) electricity, (6) chemicals (FF and MIBK), (7) ethanol (solvent used for F-ALD-1-NH₂ synthesis and catalyst regeneration), (8) catalyst (manufacture and recycling of Ru/C), and (9) process operation. For each impact category *j*, the total impact was computed as follows:

$$\text{impact}_j = \sum_i (m_i \times \text{CF}_{i,j}) \quad (1)$$

where *m_i* is the emission of substance *i* and CF_{*i,j*} its characterization factor.

2.4.3. Sensitivity Analysis. A one-at-a-time sensitivity analysis was performed to evaluate the effect of key parameters: catalyst regeneration cycles (C), overall F-ALD-1-NH₂ yield, MIBK/FF molar ratio, and ethanol/FF molar ratio.

2.4.4. Uncertainty Analysis and Confidence Interval Estimation. Uncertainty was assessed via Monte Carlo (MC) simulations (10,000 iterations) with log-normal distributions derived from the pedigree matrix approach.⁴⁶ MC simulation is the most widely used and recommended approach for uncertainty analysis in LCA and is implemented in major LCA software packages including SimaPro. The 10,000 iteration sample size is consistent with recommendations in the LCA literature for achieving stable results in comparative studies. 95% confidence intervals were derived empirically from simulation outputs. The comparative robustness between process configurations was evaluated using a discernibility analysis, where

the percentage of MC runs favoring each process was calculated. The discernibility analysis counts the number of MC realizations where one product alternative has a lower score than another, expressed as $n(A > B)$ and $n(B > A)$. The decision criterion for discernibility is that either alternative dominates the other in a statistically significant way.

A threshold of $\geq 70\%$ of MC iterations favoring one process configuration was adopted as an indicator of statistically robust superiority. This criterion provides a practical balance between statistical confidence and the uncertainty inherent to early-stage technoeconomic and life cycle assessments, allowing meaningful comparison of competing process configurations while avoiding overinterpretation of small differences within overlapping confidence intervals. This threshold is consistent with established discernibility approaches in comparative LCA literature, where the percentage of runs supporting one alternative is used to assess the robustness of conclusions in exploratory analyses. Heijungs and Kleijn note that a usual significance level is 0.95 (95%) for confirmatory analyses.⁴⁷ However, for exploratory analyses such as discernibility, researchers have used 70%, 80%, and 90% thresholds depending on the decision context. The 70% value represents a conservative balance: it is sufficiently high to indicate a clear trend, yet acknowledges the inherent uncertainty of early-stage process modeling. It is important to note that formal null hypothesis significance testing (NHST) in LCA has been critically examined, as with a large number of runs (e.g., 10,000), statistical hypotheses that should not be rejected are in fact rejected in a highly convincing way. This reinforces the appropriateness of the discernibility approach over formal hypothesis testing in this context.

Parameter uncertainties were derived from Ecoinvent data quality indicators according to the Ecoinvent report v2.2.⁴⁸ The square of geometric standard deviation for each input parameter, σ_g^2 , was computed using the expression

$$\sigma_g^2 = \exp[\ln(\sigma_0^2) + \sum_{i=1}^5 \ln(\sigma_i^2)] \quad (2)$$

where σ_1^2 , σ_2^2 , σ_3^2 , σ_4^2 , and σ_5^2 are the uncertainty factors of reliability, completeness, temporal correlation, geographical correlation, technological correlation, and sample size, and σ_0^2 is the basic uncertainty factor. Each criterion receives a score of 1 up to 5 corresponding to five quality levels for which an uncertainty factor is attributed. The uncertainty factor of sample size (σ_0^2) exists in previous versions of the pedigree matrix but is currently considered as an obsolete indicator. Accordingly, this factor was not taken into account in our calculations. The description of the quality levels and corresponding uncertainty factors for the foreground data can be found in Table S12. The scores used for the pedigree matrix for the different steps of two-step and single-reactor processes are listed in Table S13.

2.5. Technoeconomic Analysis

2.5.1. Production Costs. Full manufacturing costs (FMC) or operational expenditure (OPEX) of F-ALD-1-NH₂ was calculated as

$$\text{FMC} = \frac{\text{variable cost} + \text{fixed cost} + \text{depreciation}}{\text{annual production}} \quad (3)$$

Fixed costs included labor and maintenance; depreciation was based on a 15-year facility life. Variable costs included raw materials, catalysts, utilities, wastes, and byproducts (all based on 2018 values) (Table 1). The cost of Ru/C was based on the market Q2 2018 Ru price (€24,430/kg Ru). For both processes, four initial catalyst charges were assumed: one for the reaction, one for internal regeneration, one for external recycling, and one spare for loading. Capital (CAPEX) expenditures were estimated using Taylor's process step scoring method with an estimated error within ± 30 –40%. These estimates are based on simplified scale-up assumptions (Table S7). The CAPEX and FMC values presented in this study should therefore be interpreted as early-stage estimates suitable for comparative analysis and sensitivity studies rather than as definitive cost predictions for commercial implementation.

2.5.2. Economic Performance. A technoeconomic analysis (TEA) was conducted to produce F-ALD-1-NH₂ in single-reactor and two-reactor processes for a production scale of 3300 tons/year of F-ALD-1 over a 15-year plant lifetime with 10-year CAPEX depreciation. Cash flows, internal rate of return (IRR), and minimum selling price (MSP) were calculated using standard discounted cash flow equations.

2.5.3. Monetization of Environmental Impacts. Environmental impacts were monetized using Solvay's Sustainable Portfolio Management (SPM) framework, combining operational vulnerability (cradle-to-gate LCA) and market alignment (regulatory and market trends).^{49,50} Shadow costs were applied to quantify environmental damage in economic terms (€/kg of F-ALD-1-NH₂).⁵¹

3. RESULTS AND DISCUSSION

3.1. Technoeconomic Analysis

The economic analysis is based on industrial-scale projections derived from laboratory data using standard scale-up correlations (detailed in Table S7). While detailed flowsheeting was not performed, the approach is consistent with the early-stage TEA methodology for emerging technologies, where the objective is to identify key drivers and compare process configurations under consistent assumptions rather than to produce definitive cost estimates. The assumptions used—including 20% heat recovery efficiency, perfectly stirred mixture reactor behavior with a 1.2× safety factor, and distillation column design based on simplified vapor–liquid equilibrium—represent typical values for early-stage TEA. The sensitivity analysis in Section 3.3 systematically examines the influence of key scale-up parameters on the reported outcomes. With these considerations in mind, the following sections present the economic comparison of the two process configurations.

3.1.1. Base-Case Cost Comparison. The FMC of F-ALD-1-NH₂ differs significantly between both process configurations (Table 2). Under base-case conditions, the single-reactor process exhibits a higher FMC (€6313/ton) than the two-reactor process (€5250/ton), corresponding to an increase of approximately 17–20%. This difference is primarily driven by higher variable costs in the single-reactor configuration (€4463/ton vs €3110/ton), which account for 71% of the FMC compared to 60% in the two-reactor process. The increase in variable costs is mainly attributed to lower selectivity toward F-ALD-1-NH₂, leading to higher consumption of raw materials

Table 2. FMC of F-ALD-1-NH₂ for Base-Case Single-Reactor and Two-Reactor Processes (in €/ton)^a

	single reactor	two reactors	difference (%)
Variable cost	4477 (71%)	3144 (60%)	+30%
Fixed cost ^b	1100 (17%)	1390 (26%)	−26%
Depreciation	750 (12%)	750 (14%)	0%
FMC cost (base case 1)	6332	5250	+17%
FMC cost (best case)	3872	4287	−11%
MSP (base case 1)	7416	6208	+16%
MSP (best case)	5137	5432	−5.7%
SPM (base case 1)	7416	6208	+16%
SPM (best case)	5137	5432	−5.7%

^aProduction = 3300 tons/year of F-ALD-1-NH₂, operation = 8000 h.

^b3.0 and 4.3 shift positions for the single-reactor and two-reactor processes, respectively.

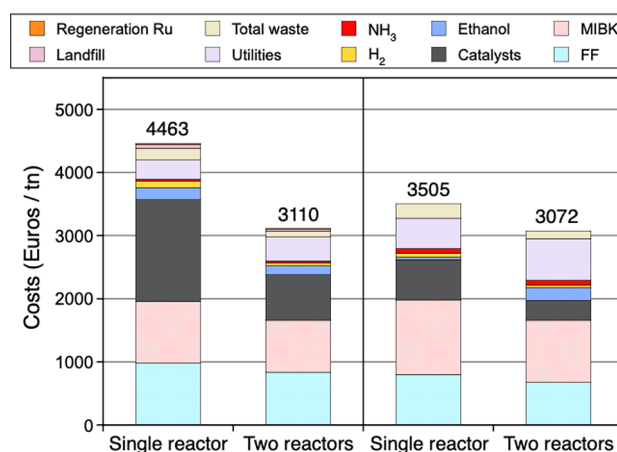
(FF, MIBK, NH₃, and H₂) per unit of product, as well as increased waste generation. In contrast, fixed costs are lower for the single-reactor process (−26%, €1100/ton vs €1390/ton), reflecting reduced labor requirements (3.0 vs 4.3 shift positions, respectively, corresponding to ~€360/ton in the former case) and simplified process operation (Table S14).

Depreciation costs are comparable in both configurations (~€750/ton), consistent with similar total capital expenditures (CAPEX). Indeed, the overall CAPEX is nearly identical for both processes (~€22.6 million), indicating that process intensification does not significantly reduce investment costs at this stage of development. A breakdown of capital costs reveals that inside battery limits (ISBL) equipment dominates in both cases, accounting for €21.3 million in the single-reactor process and €21.7 million in the two-reactor configuration. Within ISBL, the reactor represents the largest single contribution (~45% of total CAPEX), reflecting the importance of reaction and associated high-pressure equipment. The cost associated with Ru/C catalyst inventory (four initial charges for operation, regeneration, recycling, and contingency) is substantially higher in the single-reactor process (€1.30 million vs €0.67 million).

Overall, while the single-reactor configuration benefits from reduced fixed costs and operational simplification, these advantages are outweighed by higher variable costs linked to suboptimal reaction performance at base case 1 operation. This highlights that process intensification, although effective in reducing process complexity, does not inherently guarantee economic benefits and must be evaluated in conjunction with catalytic efficiency and selectivity.

3.1.2. Cost Drivers and Process Limitations. A detailed breakdown of variable costs (Figure 1) reveals that feedstocks dominate the economic performance in both configurations. FF and MIBK together represent the largest cost contributors, with higher consumption in the single-reactor process due to its lower overall yield (82% vs 70%; €837/ton vs €980/ton for FF; €822/ton vs €982/ton for MIBK). Catalyst-related costs remain comparatively modest for Ru/C (€76/ton vs €98/ton) but are significantly affected by the loading of the A26 catalyst, which is substantially higher in the single-reactor configuration (20 wt % vs 40 wt %; €644/ton vs €1508/ton). The two-reactor process incurs 43% lower variable costs overall.

These findings highlight that yield and catalyst loading are the primary economic bottlenecks for the intensified process.

**Figure 1.** Breakdown of (left) variable and (right) SPM costs for F-ALD-1-NH₂ production (base case 1) via single-reactor and two-reactor processes.

Lower selectivity and higher byproduct formation increase raw material demand and downstream processing requirements, thereby offsetting gains from process simplification.

3.1.3. Sensitivity Analysis of Variable Costs and Process Optimization. A sensitivity analysis was performed to identify the main economic drivers and optimization levers affecting the variable costs of F-ALD-1-NH₂ production. As discussed in Section 2.3.2, scale-up uncertainties are significant. The following sensitivity analysis addresses these by systematically evaluating the influence of key parameters on the economic outcomes.

The analysis considered both market-related fluctuations (i.e., prices of FF, MIBK, H₂, NH₃, ethanol, and Ru catalyst) and key process variables, including (1) overall F-ALD-1-NH₂ yield, (2) MIBK/FF molar ratio (R1), and (3) EtOH/FF molar ratio (R2). Three scenarios were defined for each process configuration: (i) base case 1, corresponding to experimentally derived conditions (74% yield for single-reactor; 91% for two-reactor; 40 and 20 wt % A26 loading, respectively); (ii) base case 2, in which the single-reactor process is aligned with the two-reactor configuration in terms of overall yield (91%) and A26 loading (20 wt %); and (iii) best case, assuming ideal performance (100% overall yield and reduced A26 loading of 5 wt %) for both processes. It is important to emphasize that the best-case scenario is a theoretical optimization exercise, not a prediction of industrial viability. This scenario serves as a prospective design objective illustrating the theoretical sustainability potential of process intensification rather than a forecast of immediately achievable industrial performance.

The main trends are summarized in Figure 2 and detailed in Figures S5, S6 and Tables S15, S16.

3.1.3.1. Fluctuation of Reactant and Catalyst Costs. Market price variability of key inputs—particularly FF, MIBK, and ruthenium—has a pronounced impact on process economics. Over the 2018–2025 period (Figures S3 and S4), these fluctuations translate into variations in variable costs ranging from −7% to +37% for the single-reactor process and −14% to +47% for the two-reactor configuration (overall 1 in Figure 2). Among these inputs, FF and MIBK dominate the cost sensitivity due to their high consumption rates, whereas the Ru/C catalyst,

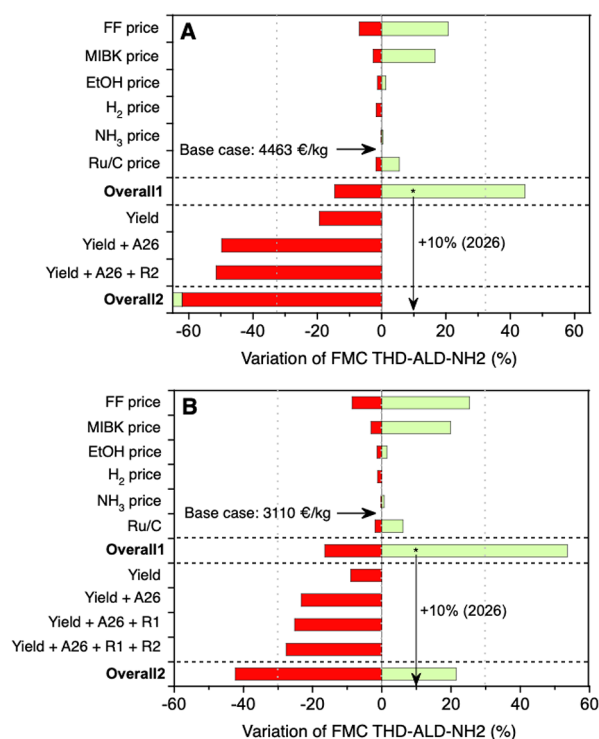


Figure 2. Sensitivity analysis for variable costs including the effect of the variability of reactant costs and chemicals (FF, MIBK, H_2 , NH_3 , and ethanol), overall yield, MIBK recycling ratio (R1), and EtOH recycling ratio (R2) influencing the FMC of F-ALD-1 for the (A) single-reactor and (B) two-reactor processes. The asterisk indicates the FMC cost using December 2025 prices for all raw materials except Ru (May 2026).

despite its high unit price, contributes more moderately to cost variability (−1.8% to +5.5% for the single-reactor and −2.0% to +6% for the two-reactor process). This reflects the relatively low catalyst make-up rate enabled by recycling and regeneration strategies.

3.1.3.2. Catalyst Lifetime and Regeneration Cycles (C). Catalyst lifetime is a critical parameter influencing both economic and environmental performance. Assuming a 90% Ru recovery efficiency during regeneration, the FMC increases sharply at low numbers of regeneration cycles due to higher fresh catalyst demand. The analysis indicates that maintaining at least three regeneration cycles per year ($C \geq 3$) is necessary to limit catalyst-related costs (Figure S6). Below this threshold, the cost penalty associated with Ru losses becomes significant, particularly for the single-reactor configuration where catalyst inventory is higher.

3.1.3.3. Impact of Overall Yield. The overall yield of F-ALD-1- NH_2 is identified as the most influential process parameter. Improving the yield of the single-reactor process from 74% (base case 1) to 91% (base case 2) results in a substantial reduction in variable costs from €4477/ton to €3607/ton (−19%), primarily due to decreased consumption of reagents and reduced byproduct formation. Despite this improvement, the single-reactor process remains more costly than the two-reactor configuration at equivalent yield (€3144/ton).

However, further optimization—specifically reducing A26 loading to 20 wt %—lowers the variable cost of the single-reactor process to €2958/ton (−34% relative to base case 1),

with a corresponding FMC of €4685/ton. Under these conditions, the single-reactor configuration becomes economically competitive and even slightly more favorable than the two-reactor process (FMC of €5284/ton).

Increasing the yield to 100% for both processes at 20 wt % A26 loading results in additional variable cost reductions of 6% (single-reactor) and 9% (two-reactor), reaching €2681/ton and €2886/ton, respectively. The resulting FMC remains lower for the single-reactor process (€4368/ton vs €4869/ton) due to its inherently lower fixed costs. However, it must be emphasized that these 100% yield conditions represent a theoretical optimum that has not been experimentally demonstrated for this system. Achieving such yields would require substantial advances in catalyst selectivity, activity, and stability, as well as optimization of reaction conditions beyond what has currently been achieved at the laboratory scale.

3.1.3.4. Effect of A26 Catalyst Loading. Catalyst loading represents another major optimization lever. Reducing A26 loading from 20–40 to 5 wt % at 100% overall yield leads to a significant decrease in variable costs to €2251/ton (single-reactor) and €2441/ton (two-reactor). This reduction translates into FMC values of €3933/ton and €4424/ton, respectively, confirming that catalyst optimization can strongly enhance the economic viability of both configurations, with a more pronounced benefit for the intensified process.

3.1.3.5. MIBK/FF Molar Ratio (R1). The MIBK/FF molar ratio primarily affects separation and recycling requirements. In the two-reactor process, excess MIBK must be separated after the aldol condensation step, increasing energy demand. At 100% overall yield and 5 wt % A26 loading, reducing R1 from 6.5 to 3.4 results in modest cost reductions (−2% in variable costs and −1% in FMC). This relatively limited impact indicates that solvent recycling efficiency is already high, and further improvements provide diminishing returns.

3.1.3.6. EtOH/FF Molar Ratio (R2). Similarly, decreasing the EtOH/FF molar ratio from 6.0–6.5 to 3.2–3.4 at 100% overall yield, 5 wt % A26 loading leads to moderate cost reductions (1–3% in variable costs and ~2% in FMC) for both configurations. The relatively small sensitivity reflects the high recycling rate of ethanol and its lower contribution to total material costs compared to FF and MIBK.

3.1.3.7. Combined Optimization and Process Comparison. When all optimization levers are applied simultaneously (100% overall yield, reduced catalyst loading, optimized solvent ratios, and more efficient recycling), the single-reactor configuration exhibits a substantially larger reduction in variable costs compared to the two-reactor process (−51% vs −26%). Under these best-case conditions, variable costs decrease to €2190/ton (single-reactor) and €2315/ton (two-reactor), corresponding to FMC values of €3872/ton and €4287/ton, respectively. At this stage, the single-reactor process becomes clearly advantageous, offering approximately 10% lower FMC and up to 15% lower capital expenditure (CAPEX), primarily due to process simplification and reduced equipment requirements.

3.1.4. Normalized Comparison at Identical Yield and Catalyst Loading. To isolate the true effect of reactor configuration from the effect of reaction performance, a normalized comparison was performed in which the single-reactor process was modeled at the same overall yield (91%) and A26 catalyst loading (20 wt %) as the two-reactor process. This analysis builds on the sensitivity scenarios already presented (base case 2) and provides a clearer picture of the intrinsic benefits

and limitations of process intensification. Under these normalized conditions (Table 3), several key observations emerge:

1. Variable costs remain higher for the single-reactor process (+15%): Even at identical yields and A26 loading, the single-reactor process incurs higher variable costs (€3600/ton vs €3144/ton for the two-reactor process). This reflects the inherent challenges of the intensified configuration, where the absence of intermediate purification necessitates higher catalyst-related requirements and may introduce additional separation burdens.
2. Fixed costs are significantly lower for the single-reactor process (−21%): The single-reactor configuration requires fewer operators (3.0 vs 4.3 shift positions), resulting in lower labor costs (€1100/ton vs €1390/ton). This represents a genuine benefit of process intensification, arising from process simplification and reduced equipment complexity.
3. The net economic effect favors the single-reactor process (−3% FMC): The lower fixed costs of the single-reactor configuration slightly outweigh its higher variable costs, resulting in a modest cost advantage of approximately 3% lower FMC (€5100/ton vs €5250/ton) at equal yields.

These results demonstrate that the apparent disadvantage of the single-reactor process under base-case conditions originates primarily from its lower catalytic performance (74% yield and 40 wt % A26 loading) rather than from the reactor configuration itself. When identical reaction performance is assumed, the intrinsic benefits of process intensification—reduced fixed costs, simplified process design, and lower operator requirements—become evident.

However, the normalized comparison also reveals that process intensification does not automatically translate into superior performance. While the single-reactor configuration offers genuine benefits in terms of fixed costs and process simplification, these advantages are partially offset by higher variable costs associated with catalyst requirements and separation burdens. The yield gap (74% vs 91%) accounts for approximately 60–70% of the observed FMC difference under

base-case conditions, while the higher A26 loading accounts for the remainder.

The sensitivity analysis confirms that the single-reactor process only becomes clearly superior (both economically and environmentally) under the best-case scenario (100% yield, 5 wt % A26), which remains a theoretical optimization target requiring substantial catalyst development. This highlights the importance of continued catalyst optimization to fully realize the potential benefits of process intensification.

3.1.5. Minimum Selling Point (MSP). A discounted cash flow analysis was performed to estimate the minimum selling price (MSP) of F-ALD-1-NH₂ production, assuming an annual capacity of 3300 tons/year, a plant lifetime of 15 years, and a target internal rate of return (IRR) of 15%.

Under base-case conditions (base case 1), the MSP is estimated at €7416/ton for the single-reactor process and €6208/ton for the two-reactor configuration (Table 2). This corresponds to ~16% higher MSP for the intensified process, indicating that, at current performance levels, the two-reactor route is economically more viable. This difference is consistent with the higher FMC observed for the single-reactor system, primarily driven by increased variable costs associated with lower selectivity and higher reagent consumption.

In contrast, under optimized conditions (best case), the economic ranking between the two configurations is reversed. The MSP decreases to €5137/ton for the single-reactor process, compared to €5432/ton for the two-reactor route, corresponding to a 5.7% reduction. This improvement reflects the greater sensitivity of the intensified process to optimization levers, particularly enhancements in overall yield and reductions in catalyst loading and solvent usage. These MSP values should therefore be interpreted as indicative of the theoretical potential of process intensification rather than as predictions of achievable industrial performance.

These results highlight that while the single-reactor configuration is initially disadvantaged due to suboptimal reaction performance, it offers greater long-term economic potential when process parameters are optimized. The transition from a cost penalty (+16%) to a cost advantage (−5.7%) underscores the

Table 3. Environmental Impact (Midpoint Categories 1–10) of Single-Reactor and Two-Reactor Processes for F-ALD-1 Production^{a,b,c}

no.	impact category	unit	single-reactor	two-reactor	diff. (%)
1	GWP 100a	kg CO ₂ -eq/kg	9.50	7.50	21%
	Trapped CO ₂ [Biogenic CO ₂]	kg CO ₂ -eq/kg	−1.19	−1.19	
2.1	Nonrenewable energy [NRE]	MJ primary/kg	163	134	18%
2.2	Renewable energy [Renew]**	MJ/kg	4.20	3.40	19%
3.1	Human toxicity potential [HTP]	kg 1,4-DB-eq/kg	3.10	2.40	23%
3.2	Freshwater aquatic ecotoxicity potential [FAETP]	kg 1,4-DB-eq/kg	2.50	1.70	32%
3.3	Marine aquatic ecotoxicity potential [MAETP]	kg 1,4-DB-eq/kg	3.106	2.033	35%
3.4	Terrestrial ecotoxicity potential [TETP]	kg 1,4-DB-eq/kg	0.0447	0.0362	19%
4	Water consumption [Water]	m ³ /kg	0.197	0.172	13%
5	Abiotic depletion potential [ADP]	kg Sb-eq/kg	0.080	0.060	25%
6	Quantitative land use [Land Use]	m ² a kg	2.01	1.71	15%
7	Acidification potential [AP]	kg SO ₂ -eq/kg	0.0428	0.0334	22%
8	Eutrophication potential [EP]	kg PO ₄ -eq/kg	0.0183	0.0139	24%
9	Ozone layer depletion potential [OLDP]	kg CFC11-eq/kg	1.08 × 10 ^{−6}	8.94 × 10 ^{−7}	17%
10	Photochemical oxidant creation potential [POCP]	kg C ₂ H ₄ -eq/kg	0.00502	0.00364	27%

^aCalculations assuming Ru/C catalyst regeneration cycles per year ($C = 3$). ^bValues for 1 kg of F-ALD-1-NH₂. ^cSee Table S17 for a breakdown of NRE (nuclear, coal, crude oil, and natural gas).

importance of integrating reaction optimization with process design when evaluating intensified systems. The MSP analysis confirms that process intensification does not inherently guarantee economic benefits but can become advantageous when key performance limitations, especially yield and catalyst efficiency, are effectively addressed.

3.2. Contribution to Environmental Impacts

The environmental impact results presented here should be interpreted with the same caveats as the TEA results. The environmental inventory is based on laboratory-scale reaction data and simplified scale-up assumptions. Uncertainty analysis (Section 3.4) provides confidence intervals for key impact categories, but the absolute values should be considered indicative rather than definitive. The primary value of this LCA lies in its comparative analysis of process configurations and identification of environmental hotspots.

3.2.1. Environmental (SPM) Costs. The monetized environmental impact, expressed as Sustainable Portfolio Management (SPM) cost, is higher for the single-reactor process (€3521/ton) than for the two-reactor configuration (€3113/ton) (Table 2), indicating a less favorable environmental performance under base-case conditions. This trend is consistent with the technoeconomic results and reflects the higher material and energy intensities associated with the intensified process at its current level of maturity.

A breakdown of SPM contributions reveals that feedstocks, primarily FF and MIBK, are the dominant contributors in both configurations, mirroring their major role in the FMC. Their impact arises from upstream burdens associated with biomass processing (for FF) and petrochemical production (for MIBK), which are amplified in the single-reactor process due to lower overall yield and higher consumption per unit of product.

In addition to raw materials, energy-related contributions (utilities) play a more prominent role in SPM costs than in the economic analysis. In particular, steam demand is a key hotspot, driven by separation and MIBK/ethanol purification steps. Approximately 65% of total steam consumption is attributed to ethanol recovery, highlighting the significant environmental burden associated with solvent handling. This contribution is slightly more pronounced in the single-reactor configuration due to increased solvent circulation and separation loads linked to byproduct formation.

In contrast, the contribution of catalysts to SPM cost remains relatively limited, despite the high economic value of ruthenium. This is primarily due to effective catalyst recycling and the relatively small mass fraction involved. The contribution from the A26 catalyst is also minor, although it becomes more relevant at high loadings.

The main levers identified for reducing FMC, namely, feedstock consumption, overall yield improvement, and reduction of A26 loading, also directly translate into lower environmental costs. This alignment indicates that economic and environmental objectives are largely synergistic in this system. Overall, these results emphasize that the environmental performance of the single-reactor process is highly sensitive to reaction efficiency and downstream processing requirements. While this configuration currently exhibits a higher SPM cost, it retains significant potential for improvement through process optimization, particularly by reducing material losses and energy demand associated with separation steps.

3.2.2. Environmental Impact Comparison. Table 3 summarizes the environmental impacts of the single-reactor and two-reactor configurations for F-ALD-1-NH₂ production under base-case conditions (base case 1). The single-reactor process exhibits systematically higher impacts across all mid-point categories compared to the two-reactor configuration. The largest relative increases are observed for freshwater and marine ecotoxicity ([FAETP] +32% and [MAETP] +35%), followed by photochemical oxidant creation ([POCP] +27%), abiotic depletion ([ADP] +25%), eutrophication ([EP] +24%), human toxicity ([HTP] +23%), acidification ([AP] +22%), and global warming potential ([GWP 100a] +21%). Smaller but still significant increases are observed for nonrenewable energy demand ([NRE] +18%), renewable energy use (+19%), land use (+15%), water consumption (+13%), and ozone layer depletion ([OLDP] +17%). These higher impacts are primarily attributed to the lower overall yield of the single-reactor process and higher A26 catalyst loading required, which together increase material consumption and waste generation per unit of product. As a result, upstream burdens associated with feedstock production, solvent use, and energy demand are amplified.

3.2.2.1. Contribution Analysis: Identification of Partial Benefits. Despite its overall higher impact, the contribution analysis (Figure 3) reveals several partial environmental benefits of the single-reactor configuration when examining individual process contributors.

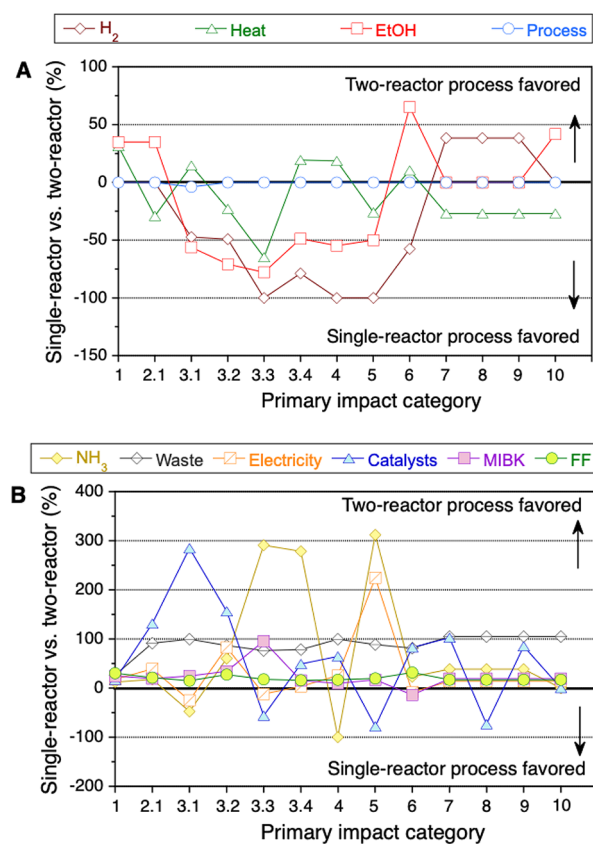


Figure 3. (A, B) Relative impacts between the single-reactor and two-reactor processes (base case 1 for both processes). The different impact categories for each reference (from 1 to 10) are listed in Table 3.

Ethanol shows substantially lower contributions in the single-reactor process across multiple categories, including [Land Use] (−78%), [ADP] (−71%), [Water] (−55%), [EP] (−55%), [OLDP] (−50%), and [AP] (−49%). This reflects reduced solvent handling and/or more efficient integration of reaction and separation steps, limiting the environmental burden associated with ethanol production and recycling.

Heat (steam demand) also exhibits moderate reductions ($\approx -23\%$ to -29%) across several categories, including [NRE], [HTP], [FAETP], [MAETP], [TETP], and [OLDP]. These reductions suggest that, despite higher overall impacts, the intensified process can partially decrease energy requirements in specific unit operations, likely due to process integration and reduced intermediate handling.

Hydrogen contributes less to most impact categories in the single-reactor process, with particularly strong reductions for [Land Use] (−100%), [EP] (−100%), [AP] (−79%), and [POCP] (−58%). This indicates more efficient hydrogen utilization under tandem conditions, although the overall process performance remains limited by yield.

Interestingly, catalysts, despite being used in larger quantities in the single-reactor process, show lower contributions to certain categories such as [OLDP] (−78%), [FAETP] (−74%), and [Land Use] (−56%). This counterintuitive result reflects differences in catalyst life cycle inventories and recycling assumptions, highlighting that catalyst mass alone is not the dominant driver of environmental impact.

Ammonia also shows reduced contributions in specific categories, notably [EP] (−100%) and [Water] (−48%), although its overall influence remains limited compared to major contributors such as FF and MIBK.

3.2.2.2. Dominant Contributors across Impact Categories. For both configurations, the main contributors to [GWP 100a] and [NRE] are similar (Figure 4), with MIBK ($\sim 26\%$), heat utilities ($\sim 22\%$), catalysts ($\sim 18\%$), and waste treatment ($\sim 17\%$) dominating. This indicates that the difference between the two processes arises more from magnitude (i.e., higher consumption) than from fundamentally different impact sources. A similar pattern is observed for [Water], [ADP], [Land Use], [AP], [EP], [OLDP], and [POCP]

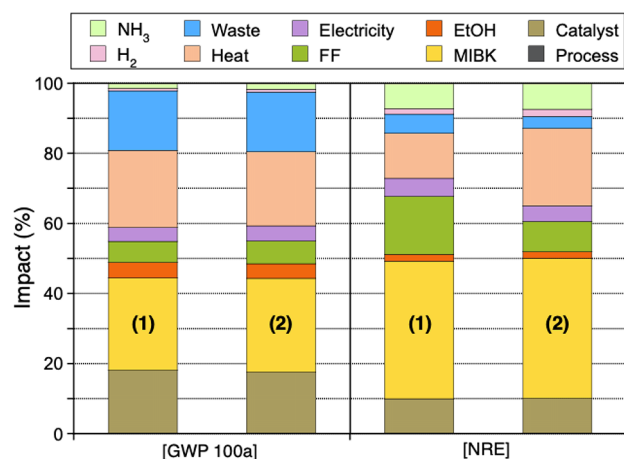


Figure 4. Impact score breakdown for global warming potential [GWP 100a] and nonrenewable energy [NRE] for (1) single-reactor and (2) two-reactor processes.

(Figure 5), where the same key contributors dominate both configurations:

- FF is the primary contributor to [Water] (61%), [Land Use] (96%), [AP] (41%), and [EP] (55%), reflecting the significant upstream impacts associated with biomass cultivation and processing.
- MIBK strongly influences [ADP] (39%) and [OLDP] (42%) due to its fossil-based origin and associated resource depletion.
- Catalysts and waste treatment contribute significantly to [AP], [EP], and [OLDP], depending on the category.
- POCP is mainly driven by waste (30–40%), followed by catalysts (16–18%) and ammonia ($\sim 12\%$), with a slightly higher contribution from process operations in the two-reactor configuration (9% vs 2%).

Details on the statistical significance of these results are provided below (see Section 3.4).

For ecotoxicity-related categories ([HTP], [FAETP], [MAETP], and [TETP]), the contribution patterns are also similar for both configurations (Figure 6).

- FF is the dominant contributor, accounting for $\sim 50\%$ ([HTP]), 37% ([FAETP]), 22% ([MAETP]), and 75% ([TETP]), confirming the strong influence of biomass-derived feedstock production on toxicity-related impacts.
- Ethanol contributes significantly to [FAETP] (23%) and [TETP] (15%), reflecting solvent-related emissions.
- Catalysts play a notable role in [HTP] (16%) and [MAETP] (30%).
- Waste treatment contributes substantially to [HTP] (12%), [FAETP] (29%), and [MAETP] (31%).

The similarity in contribution profiles between the two configurations indicates that differences in total impacts are primarily driven by scale effects (i.e., higher consumption and lower efficiency) rather than changes in impact structure.

While the absolute environmental impacts of the F-ALD-1- NH_2 production process would vary with different FF feedstocks, the comparative ranking between the single-reactor and two-reactor configurations is expected to remain unchanged. The key drivers of the difference between the two configurations—overall reaction yield, catalyst loading, and solvent requirements—are intrinsic to the reaction chemistry and process design, not to the FF supply chain. Feedstock variation would primarily shift the absolute magnitude of the upstream burdens (particularly land use, water consumption, and eutrophication) but would not alter the conclusion that the single-reactor process requires substantial optimization in yield and catalyst loading to become economically and environmentally competitive. For example, if sugarcane bagasse were used as the FF feedstock instead of corncobs, the absolute GWP, land use, and eutrophication impacts would decrease due to the waste-derived nature of the feedstock (avoiding cultivation-related burdens), while the relative difference between the two reactor configurations would remain similar because both processes would benefit equally from the reduced upstream burdens. Conversely, if

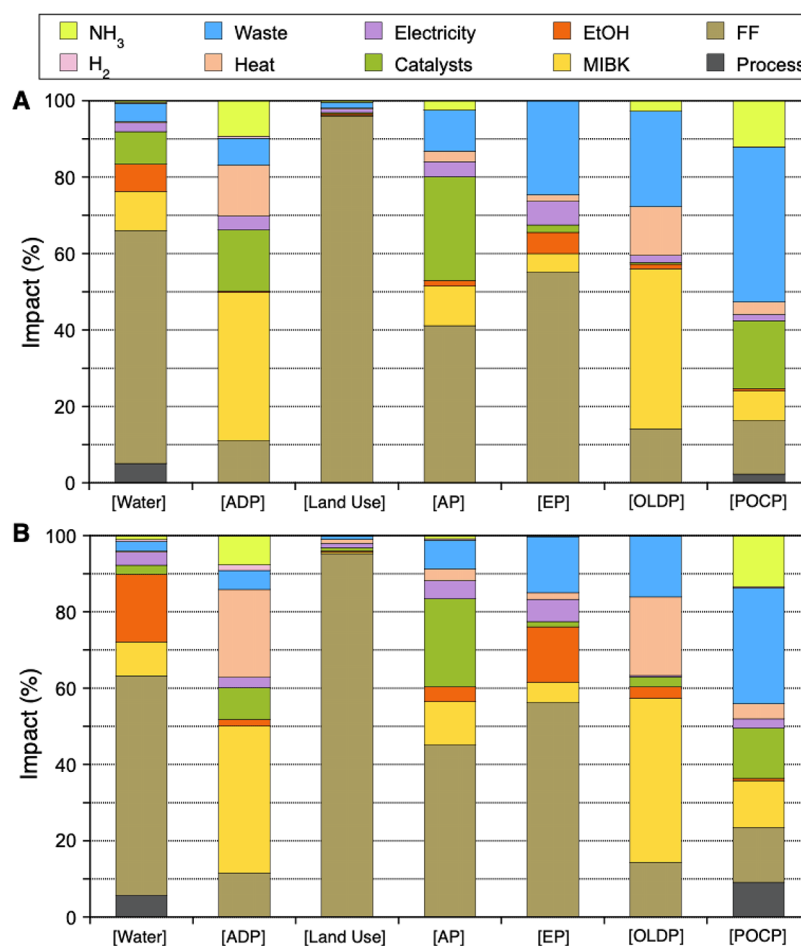


Figure 5. Impact score breakdown for water consumption [Water], abiotic depletion potential [ADP], quantitative land use [Land Use], acidification potential [AP], eutrophication potential [EP], ozone layer depletion potential [OLDP], and photochemical oxidant creation potential [POCP] for (A) single-reactor and (B) two-reactor processes.

wheat straw or corn stover were used, the increased feedstock requirement (due to lower xylose content) would amplify the upstream impacts across both configurations without changing the comparative ranking. Therefore, while the absolute values of the environmental impact categories may vary with feedstock choice, the central conclusion—that process intensification requires optimization to deliver sustainability benefits—is robust across different biomass supply chains.

To further investigate the drivers of the dominant furfural-related burdens, the furfural supply chain was decomposed into its main stages. These include: (i) corncob cultivation and harvesting, (ii) feedstock transportation, (iii) acid hydrolysis, (iv) furfural dehydration, (v) product separation and purification, and (vi) waste treatment. Based on literature evidence from LCA studies on furfural production, the following stage-level contributions were identified:

- Land use and water consumption are dominated by the cultivation stage (maize production for corncob collection), primarily due to land occupation and irrigation requirements (88–93% of water consumption).
- Eutrophication is driven by both the cultivation stage (fertilizer application leading to nitrate and phosphate

runoff) and the purification stage (distillation wastewater containing organic effluents).

- Acidification is primarily attributed to the purification stage (steam generation for distillation releasing SO_2 , SO_x , and NO_x) and the hydrolysis stage (sulfuric acid consumption).
- Human toxicity and ecotoxicity are mainly driven by acid consumption during hydrolysis (sulfuric acid is the main contributor to human toxicity and ecotoxicity) and steam generation during purification, with solvent use also contributing.
- Global warming potential is dominated by the purification stage, where steam generation for distillation accounts for the largest share of emissions (over 55% on average across most categories).

This stage-level analysis confirms that the dominant burdens are associated with feedstock cultivation, acid hydrolysis, and energy-intensive separation steps. The findings provide clear targets for process optimization: (i) reducing acid consumption in hydrolysis to lower toxicity and ecotoxicity; (ii) improving energy integration in distillation to lower GWP, AP, and

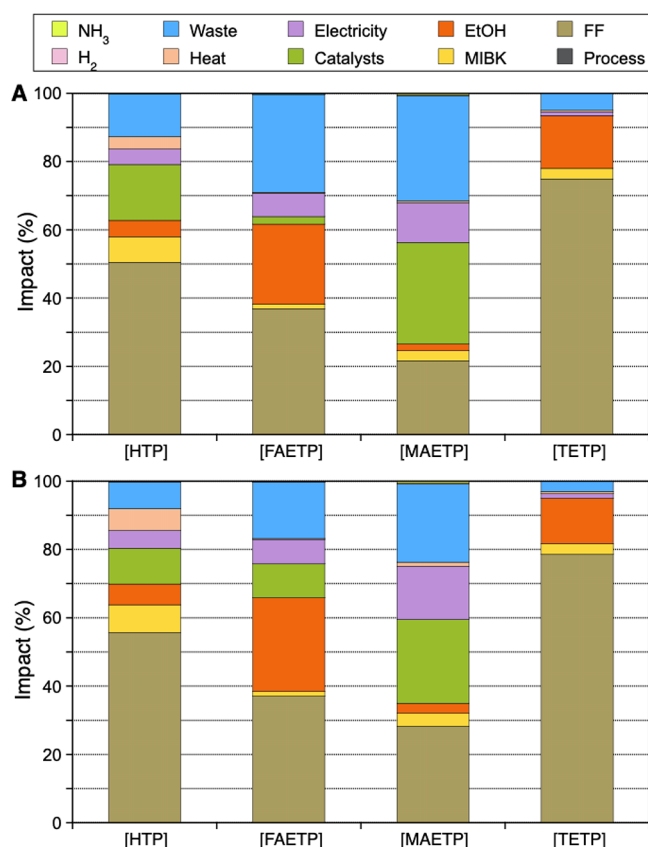


Figure 6. Impact score breakdown for human toxicity potential [HTP], freshwater aquatic ecotoxicity potential [FAETP], marine aquatic ecotoxicity potential [MAETP], and terrestrial ecotoxicity potential [TETP] for (A) single-reactor and (B) two-reactor processes.

POCP; and (iii) feedstock choice or cultivation practices to lower land use, water, and eutrophication.

3.2.2.3. Key Insight. Overall, the LCIA results demonstrate that the single-reactor (intensified) process is currently penalized across all environmental categories due to lower reaction efficiency and higher catalyst loading. However, the contribution analysis reveals important localized benefits (e.g., reduced ethanol, hydrogen, and partial energy impacts), suggesting that process intensification can deliver environmental advantages at the unit-operation level.

These findings reinforce the conclusion that the environmental performance of intensified systems is highly dependent on achieving high yields and optimized operating conditions. Without such improvements, the benefits of process integration remain insufficient to offset increased material and energy demands.

3.3. Sensitivity Analysis

A sensitivity analysis was performed to evaluate the influence of the key process parameters on the environmental performance of both configurations across all midpoint impact categories. The parameters investigated include: (1) the number of Ru/C catalyst regeneration cycles, (2) the overall F-ALD-1-NH₂ yield, (3) the A26 catalyst loading, (4) the MIBK/FF molar ratio, and (5) the ethanol/FF molar ratio. The analysis was conducted for both base-case and optimized scenarios, with detailed results provided in Tables S18 and S19.

3.3.1. Effect of the Number of Ru/C Catalyst Regeneration Cycles. The number of Ru/C catalyst regeneration cycles (C) has a dominant influence on environmental performance. Increasing C leads to a systematic and substantial rise in all impact categories for both process configurations relative to the base case 1 ($C = 3$), with particularly pronounced effects observed for toxicity- and resource-related indicators.

The most significant relative increases are observed for [GWP 100a], [FAETP], [MAETP], [TETP], [Water], [EP], [OLDP], and [POCP], with increases by more than 40% when C raises from 3 to 30 and by over 400% when C reaches 300 (Figure 7). These trends are broadly similar for both process configurations; however, slightly higher increases are observed for the two-reactor process in selected categories, particularly [GWP 100a] and [Water]. For instance, at $C = 300$, [GWP 100a] increases by approximately 341–1670%, while [Water] rises by 289–554% depending on the configuration. Such dramatic increases render both processes environmentally unfeasible at high regeneration frequencies, even at moderate values ($C \geq 30$). This highlights that the catalyst lifetime and regeneration strategy are critical bottlenecks for sustainable process design.

While catalyst regeneration is generally expected to reduce fresh catalyst demand, the environmental detriment at higher cycle numbers arises from the cumulative burden of the regeneration process itself (Table S11). Each regeneration cycle for the single-reactor process consumes 0.040 ethanol per kg F-ALD-1-NH₂ and generates the same amount of organic waste for each Ru/C catalyst regeneration cycle, with these burdens accumulating linearly with the number of cycles. At $C = 300$, for example, cumulative ethanol consumption and organic waste reaches 12 kg ethanol per kg Ru/C. These cumulative burdens eventually outweigh the avoided burden of fresh Ru/C production. Based on the cumulative inventory flows, the break-even point occurs at approximately 10–15 regeneration cycles. Beyond this point, the cumulative environmental burden of regeneration exceeds the avoided burden of fresh Ru/C production.

Uncertainty analysis based on Monte Carlo simulations confirms that the observed trends are statistically significant (95% confidence level) for key impact categories, including

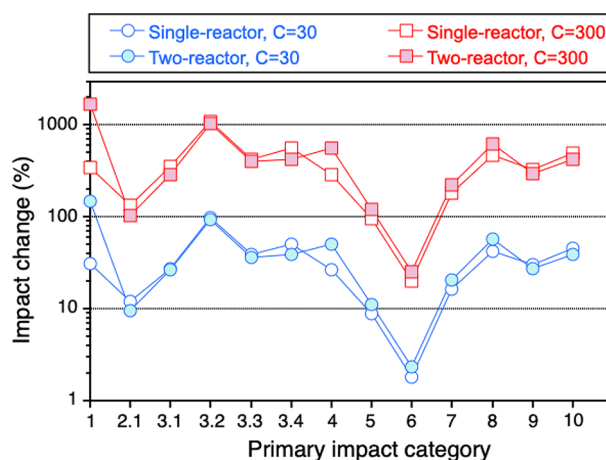


Figure 7. Impact change compared to base case 1 as a function of the number of Ru/C catalyst regeneration cycles for the single-reactor and two-reactor processes. The different impact categories for each reference (from 1 to 10) are listed in Table 3.

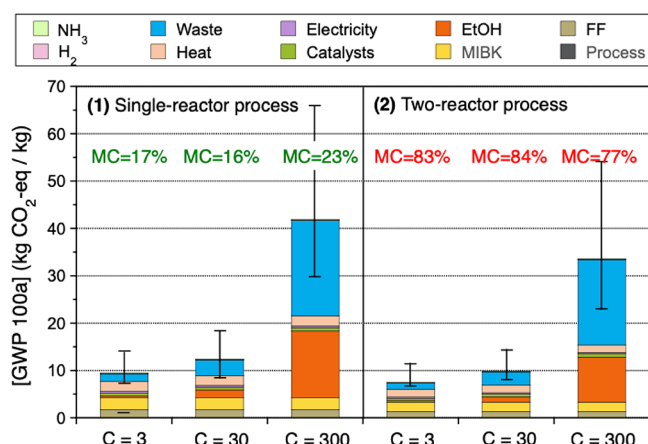


Figure 8. Effect of the number of regeneration cycles (C) for the Ru/C catalyst on global warming potential [GWP 100a] for (1) single-reactor and (2) two-reactor processes. The error bars (for a 95% confidence interval) were estimated using MC simulations.

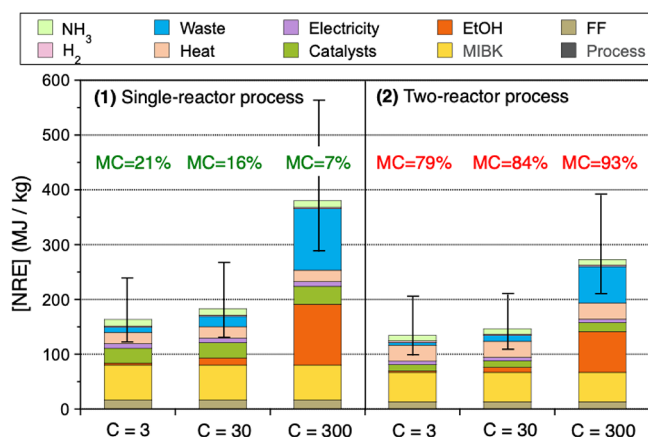


Figure 9. Effect of the number of regeneration cycles (C) for the Ru/C catalyst on nonrenewable energy [NRE] for (1) single-reactor and (2) two-reactor processes. The error bars (for a 95% confidence interval) were estimated using MC simulations.

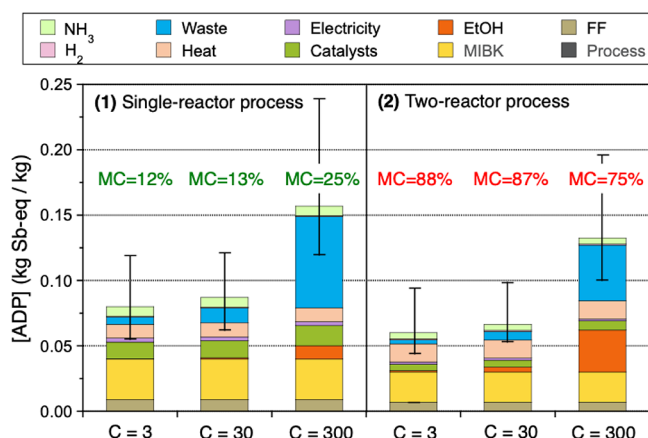


Figure 10. Effect of the number of regeneration cycles (C) for the Ru/C catalyst on abiotic depletion potential [ADP] for (1) single-reactor and (2) two-reactor processes. The error bars (for a 95% confidence interval) were estimated using MC simulations.

[GWP 100a], [NRE], [ADP], [OLDP], [POCP], and [MAETP] (Figures 8–13). The main drivers behind these increases are

- ethanol consumption associated with catalyst regeneration steps and
- waste generation and treatment, particularly from regeneration and solvent handling.

These contributions dominate the environmental burden as regeneration frequency increases, outweighing the benefits of catalyst reuse. The impacts of other categories are compiled in the Supporting Information (Figures S7–S13).

Overall, these results demonstrate that high catalyst regeneration is environmentally counterproductive, despite its intended role in reducing fresh catalyst demand. From both environmental and economic perspectives, the number of regeneration cycles should be strictly limited. Based on this analysis, a value of $C = 3$ represents a realistic and sustainable compromise and is therefore retained as the reference condition for subsequent sensitivity analyses (section 3.3.2).

3.3.2. Effect of the Overall Yield, A26 Loading, MIBK/FF, and EtOH/FF Molar Ratios. Under base-case conditions (base case 1), the single-reactor process exhibits systematically higher environmental impacts across all midpoint categories compared to the two-reactor configuration (Figures 14–18 and Figures S14–S21). This difference is primarily attributed to two factors: (i) the lower overall yield, which increases material consumption and waste generation, and (ii) the higher A26 catalyst loading required to achieve sufficient activity in the aldol condensation step.

Improving the overall yield of the single-reactor process while maintaining a high A26 loading (40 wt %) leads to a substantial reduction in environmental impacts across all categories, with decreases ranging from 19% to 25% relative to base case 1. This improvement is mainly driven by a reduced formation of byproducts and, consequently, lower waste treatment requirement. A further reduction in A26 loading from 40 to 20 wt % (base case 2) results in an additional decrease in environmental impacts. The effect is more pronounced for resource- and toxicity-related categories, including [NRE], [ADP], [AP], [POCP], [HTP], and [MAETP], with reductions of 7–12%,

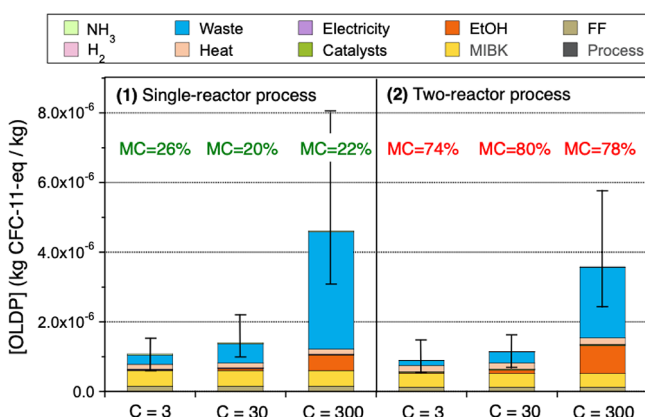


Figure 11. Effect of the number of regeneration cycles (C) for the Ru/C catalyst on ozone layer depletion potential [OLDP] for (1) single-reactor and (2) two-reactor processes. The error bars (for a 95% confidence interval) were estimated using MC simulations.

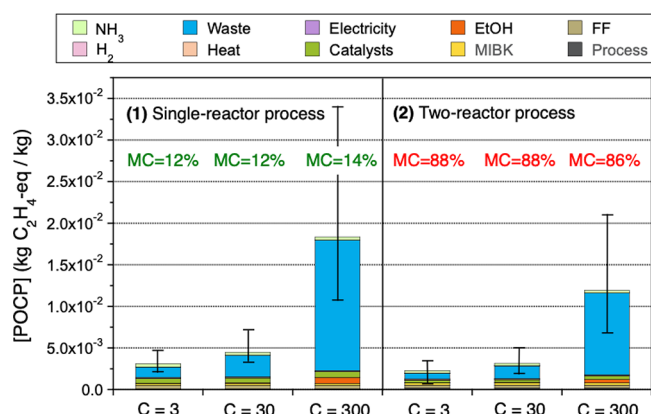


Figure 12. Effect of the number of regeneration cycles (C) for the Ru/C catalyst on photochemical oxidant creation potential [POCP] for (1) single-reactor and (2) two-reactor processes. The error bars (for a 95% confidence interval) were estimated using MC simulations.

whereas more moderate decreases (2–6%) are observed for [GWP 100a], [Water], [EP], [OLDP], [FAETP], and [TETP]. No significant change is observed for [Land Use], which remains dominated by upstream biomass production (i.e., FF feedstock). This improvement is primarily attributed to ~60% reduction in catalyst-related contributions, which significantly affects categories sensitive to metal extraction

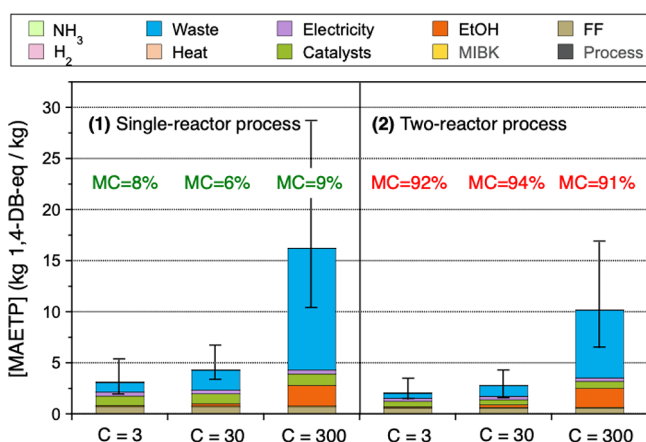


Figure 13. Effect of the number of regeneration cycles (C) for the Ru/C catalyst on maritime aquatic ecotoxicity potential [MAETP] for (1) single-reactor and (2) two-reactor processes. The error bars (for a 95% confidence interval) were estimated using MC simulations.

and processing. In addition, an ~40% decrease in waste generation contributes to further reductions, particularly in [GWP 100a], [EP], [OLDP], [POCP], [HTP], and [FAETP] (Figures S22–S34). Other contributions decrease more moderately (typically 16–19%), reflecting the distributed nature of process inputs.

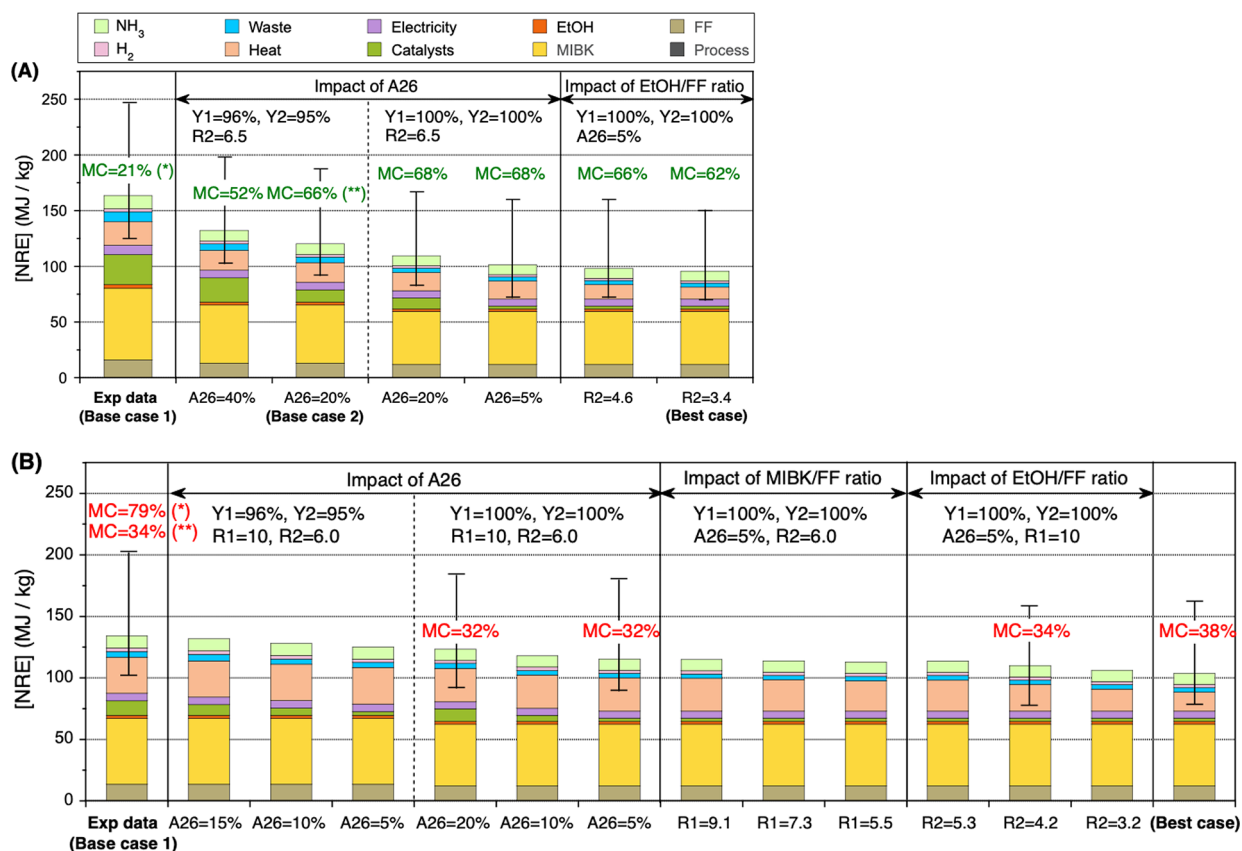


Figure 14. (A, B) Effect of the overall yield and MIBK/FF molar ratio on nonrenewable energy [NRE] for (1) single-reactor and (2) two-reactor processes ($C = 3$). The error bars (for a 95% confidence interval) were estimated using MC simulations. The numbers on top of the bars correspond to successful MC runs favoring each process (single-reactor, in green; two-reactor, in red). Nomenclature: (*) comparison of base case 1 scenarios for both processes; (**) comparison of base case 1 for the two-reactor process and base case 2 for the single-reactor process.

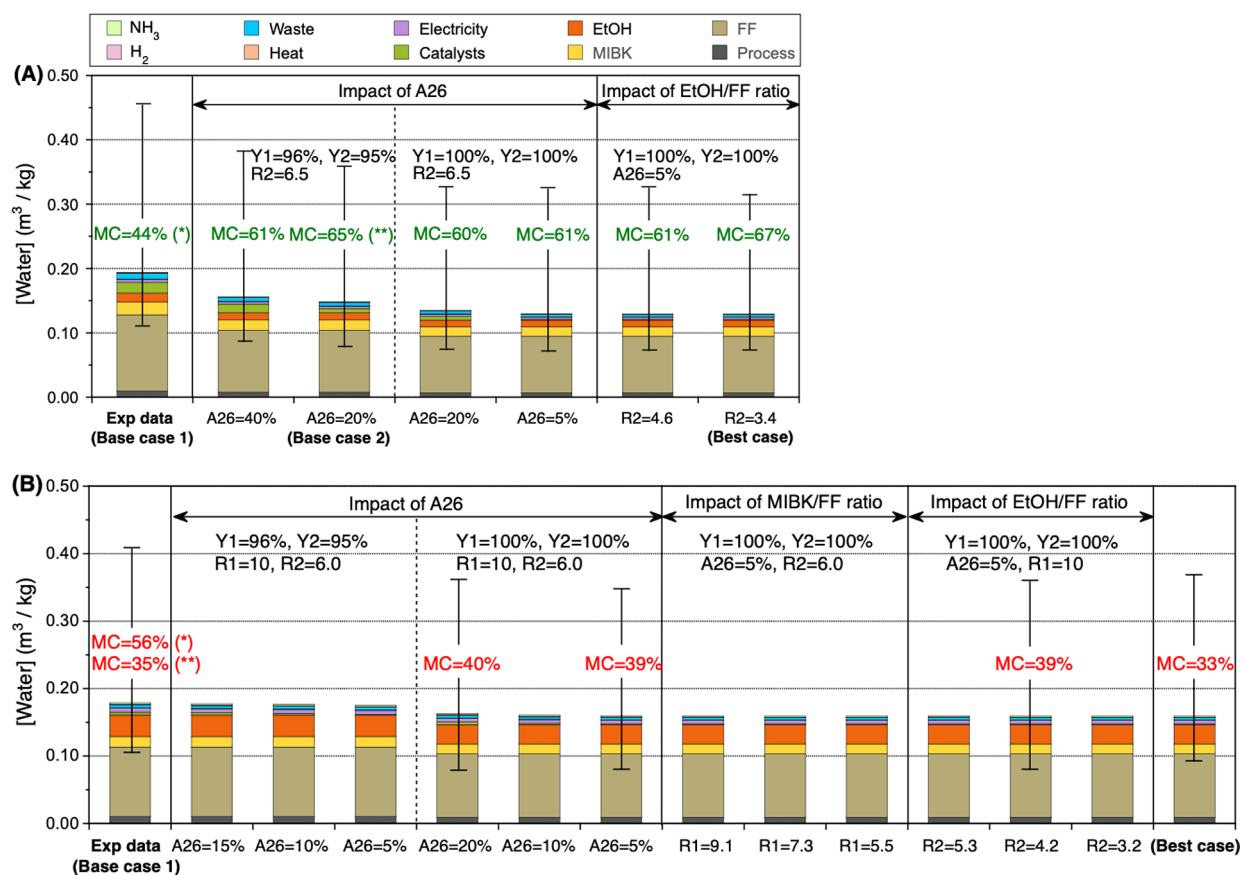


Figure 15. (A, B) Effect of the overall yield and MIBK/FF molar ratio on water consumption [Water] for (1) single-reactor and (2) two-reactor processes ($C = 3$). The error bars (for a 95% confidence interval) were estimated using MC simulations. The numbers on top of the bars correspond to successful MC runs favoring each process (single-reactor, in green; two-reactor, in red). Nomenclature: (*) comparison of base case 1 scenarios for both processes; (**) comparison of base case 1 for the two-reactor process and base case 2 for the single-reactor process.

For both process configurations, increasing the overall yield to 100% at 20 wt % A26 loading leads to further environmental improvements. Waste generation is reduced by approximately 20% for the single-reactor process and 14% for the two-reactor process, resulting in additional decreases of 7–9% across most impact categories (Figures S22–S34).

Process intensification benefits become more evident under fully optimized (best-case) conditions, combining high yield, low catalyst loading (5 wt % A26), and optimized solvent ratios. In particular, reducing the MIBK/FF molar ratio (e.g., from 10 to 5.5 in the two-reactor process) and the ethanol/FF molar ratio (from 6.5 to 3.4 for both processes) significantly lowers the environmental burden associated with separation and recycling steps. Under these conditions, the contributions of key drivers are markedly reduced:

- Catalysts: –76% (single-reactor) and –73% (two-reactor)
- Heat demand (steam and cooling for distillation): –33% and –43%
- Waste treatment: –14% and –12%
- Hydrogen consumption: –5% and –10%

Changes in other contributions remain marginal (<2%), indicating that these parameters specifically target the dominant environmental hotspots.

Overall, under best-case conditions, the single-reactor process becomes environmentally advantageous, showing reductions of up to 13–20% for key categories such as [NRE], [HTP], [TETP], [Water], [ADP], [Land Use], and [EP] compared to the two-reactor process (Figure 19). Smaller but consistent improvements (5–10%) are observed for the remaining categories.

These results clearly demonstrate that process intensification alone does not guarantee environmental benefits. Instead, its success critically depends on achieving comparable yields and optimized catalyst loadings. When these conditions are met, the integration of reaction steps into a single reactor effectively reduces material and energy demands, leading to improved environmental performance. More broadly, this analysis highlights that reaction performance (yield and selectivity), catalyst efficiency, and solvent management are the primary levers governing sustainability outcomes. Consequently, process optimization and catalyst design are as important as reactor configuration in minimizing the environmental footprint of F-ALD-1-NH₂ production.

3.4. Uncertainty Analysis

An uncertainty analysis was conducted to evaluate the statistical robustness of the environmental impact results and the comparative performance of the single-reactor and

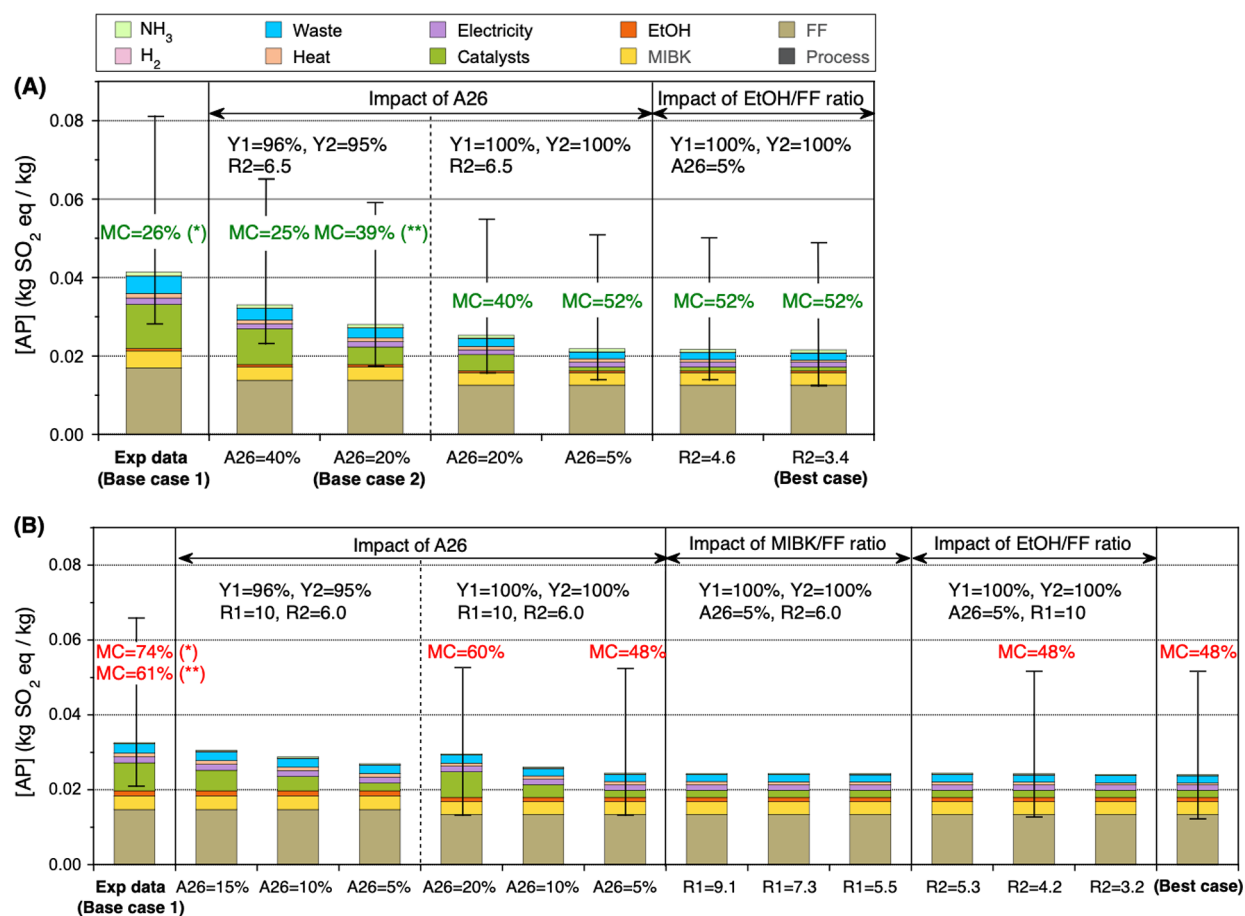


Figure 16. (A, B) Effect of the overall yield and MIBK/FF molar ratio on acidification potential [AP] for (1) single-reactor and (2) two-reactor processes ($C = 3$). The error bars (for a 95% confidence interval) were estimated using MC simulations. The numbers on top of the bars correspond to successful MC runs favoring each process (single-reactor, in green; two-reactor, in red). Nomenclature: (*) comparison of base case 1 scenarios for both processes; (**) comparison of base case 1 for the two-reactor process and base case 2 for the single-reactor process.

two-reactor processes. MC simulations (10,000 iterations) were used to propagate uncertainty in the life cycle inventory data, with results expressed as probability distributions for each impact category.

Based on the sensitivity analysis, four impact categories were identified in which the single-reactor process shows potential environmental advantages under selected conditions (i.e., $\geq 70\%$ of MC runs favoring the single-reactor configuration): [NRE], [Water], [POCP], and [FAETP] (Figure 20, $C = 3$). A complete overview of MC results for all categories and scenarios is provided in Figures S35–S38, while the corresponding log-normal distributions comparing both scenarios are plotted in Figures S39–S41.

Despite the relatively large uncertainty ranges (as reflected by wide confidence intervals), the MC analysis enables statistically meaningful comparisons between both process configurations. Under base case 1 conditions, the two-reactor process is consistently favored, with $>73\text{--}95\%$ of MC runs indicating lower impacts for most categories. Exceptions are observed for [Water], [EP], and [TETP], where differences are not statistically significant or show weaker preference (Figure S35). These results confirm the robustness of the base-case conclusion that the two-reactor configuration is environmentally preferable under nonoptimized conditions.

When comparing base case 1 for the two-reactor process with base case 2 for the single-reactor process (i.e., improved yield and reduced A26 loading), the outcome shifts in favor of the single-reactor configuration for several categories. In particular, statistically significant advantages ($\geq 70\text{--}85\%$ MC runs) are observed for [NRE], [OLDP], and [FAETP] (Figure S36), indicating that process optimization can effectively reverse the initial environmental disadvantage of the intensified system.

Under fully optimized conditions (100% overall yield and 20 wt % A26 loading), the single-reactor process consistently outperforms the two-reactor configuration across multiple categories (Figures S37 and S38). Under these conditions, the probability distributions show a clear shift toward lower impact values for the single-reactor process, with $\geq 70\text{--}89\%$ of MC runs favoring the single-reactor configuration, confirming that the environmental benefits of process intensification become statistically robust when key performance parameters are optimized. The corresponding confidence intervals for key impact categories are presented in Figures 8–18.

Overall, this analysis highlights two important points. First, uncertainty does not alter the main conclusions, as the relative ranking of process configurations remains consistent within each

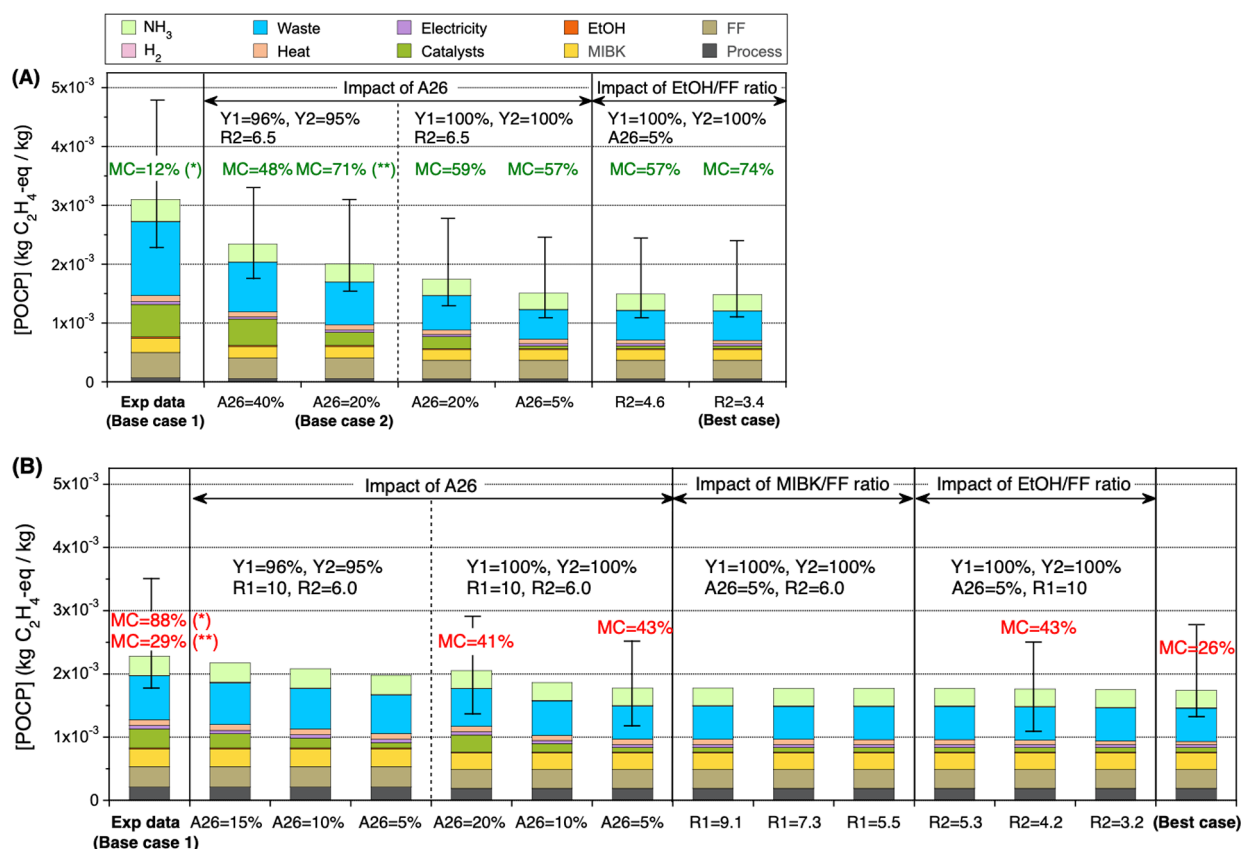


Figure 17. Effect of the overall yield and MIBK/FF molar ratio on photochemical oxidant creation potential [POCP] for (1) single-reactor and (2) two-reactor processes ($C = 3$). The error bars (for a 95% confidence interval) were estimated using MC simulations. The numbers on top of the bars correspond to successful MC runs favoring each process (single-reactor, in green; two-reactor, in red). Nomenclature: (*) comparison of base case 1 scenarios for both processes; (**) comparison of base case 1 for the two-reactor process and base case 2 for the single-reactor process.

scenario. Second, and more importantly, it demonstrates that the environmental superiority of process intensification is conditional rather than intrinsic. While the two-reactor process is more robust under base-case conditions, the single-reactor configuration becomes statistically favored once yield, catalyst loading, and solvent use are optimized. These findings reinforce the importance of combining process design with catalyst performance optimization and confirm that uncertainty-aware LCA is essential for supporting reliable decision-making in early-stage process development.

4. CONCLUSIONS

This study provides a comprehensive comparison of single-reactor and two-reactor catalytic routes for F-ALD-1-NH₂ production from biomass-derived furfural. Under base-case conditions, the two-reactor process is economically and environmentally preferred, with 16–20% lower full manufacturing cost and consistently lower impacts across all midpoint categories, driven by its higher yield (91% vs 74%) and lower catalyst loading.

However, process intensification becomes advantageous under optimized conditions—higher yield, lower catalyst loading, and optimized solvent ratios—achieving up to 10% lower cost and 5–20% lower environmental impacts. These optimized conditions remain to be demonstrated experimentally and

require further catalyst development; they should be interpreted as a prospective design objective guiding catalyst development priorities, not as a prediction of immediately achievable industrial performance.

Key drivers across both configurations include feedstock consumption, catalyst loading, regeneration efficiency, and separation energy demand. Catalyst-related parameters constitute a strong link between economic and environmental performance, highlighting that catalyst optimization should be considered a key strategy for enhancing overall process sustainability. Uncertainty and sensitivity analyses confirm the robustness of the main conclusions and demonstrate that the environmental superiority of intensified processes is conditional rather than intrinsic.

This work illustrates that sustainability advantages of intensified processes cannot be assumed a priori but must be quantitatively demonstrated through early-stage integration of TEA and LCA. The results presented here are intended to provide directional guidance for research priorities, not definitive cost or impact projections for commercial implementation. Pilot-scale validation is required to confirm scalability and refine cost and impact estimates. More broadly, the trends identified are expected to be broadly applicable to intensified catalytic processes involving tandem reactions, highlighting that success depends on simultaneously optimizing reaction efficiency, catalyst utilization, and downstream separation requirements.

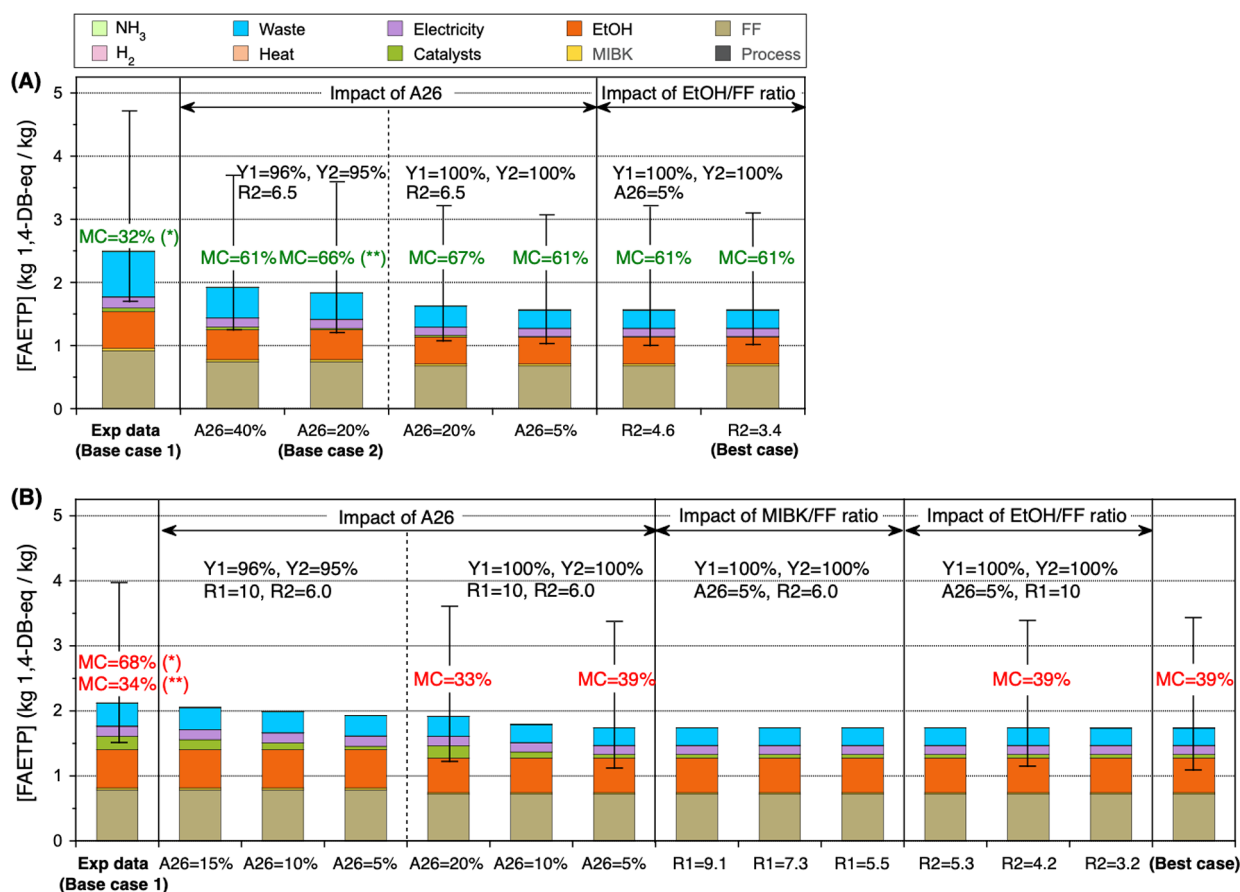


Figure 18. Effect of the overall yield and MIBK/FF molar ratio on freshwater aquatic ecotoxicity potential [FAETP] for (1) single-reactor and (2) two-reactor processes ($C = 3$). The error bars (for a 95% confidence interval) were estimated using MC simulations. The numbers on top of the bars correspond to successful MC runs favoring each process (single-reactor, in green; two-reactor, in red). Nomenclature: (*) comparison of base case 1 scenarios for both processes; (**) comparison of base case 1 for the two-reactor process and base case 2 for the single-reactor process.

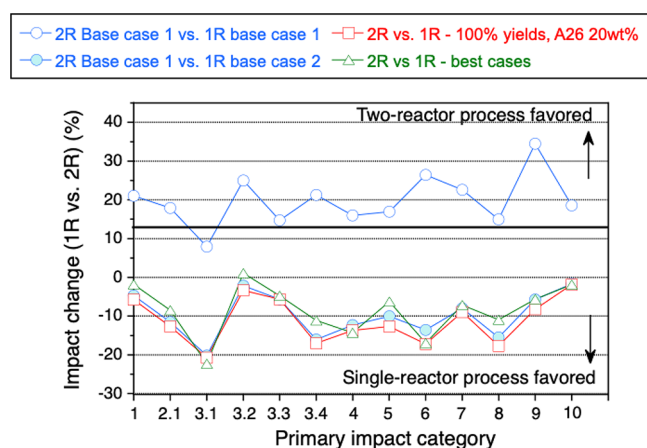


Figure 19. Relative variation of the environmental impacts between the single-reactor and two-reactor processes for different scenarios. The different impact categories for each reference (from 1 to 10) are listed in Table 3.

■ ASSOCIATED CONTENT

Data Availability Statement

All relevant data supporting the findings of this study are available within the article and its Supporting Information (SI). Additional raw data are available from the corresponding author upon reasonable request.

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acssuschemeng.6c04070>.

Flowsheets for single-reactor and two-reactor processes; market price of FF, MIBK, H_2 , and ethanol; market price of Pt, Pd, and Ru catalysts; effect of the reaction yield, A26 loading, and MIBK/FF and EtOH/FF molar ratios on FMC and breakdown of costs; breakdown of FMC and variable costs against the number of regeneration cycles (C) of Ru/C; effect of the number of regeneration cycles for Ru/C on [Water], [Land Use], [AP], [EP], [HTP], [FAETP], and [TETP]; effect of A26 loading and MIBK/FF and ethanol/FF molar ratios on [GWP 100], [ADP], [Land Use], [AP], [OLDP], [HTP], [MAETP], and [TETP]; impact score breakdown as a function of the overall yield, A26 loading, and MIBK/FF and EtOH/FF molar ratios for [GWP 100a], [NRE], [Water], [ADP], [Land Use], [AP], [EP], [OLDP], [POCP], [HTP], [FAETP], [MAETP], and [TETP]; uncertainty analysis for the different impact categories, for base case 1 for both processes, and for base case 1 for the two-reactor process and base case 2 for the single-reactor process; uncertainty analysis for $Y1 = 100\%$, $Y2 = 100\%$, and 20 wt % A26 for both processes; uncertainty analysis for best-case scenarios for both

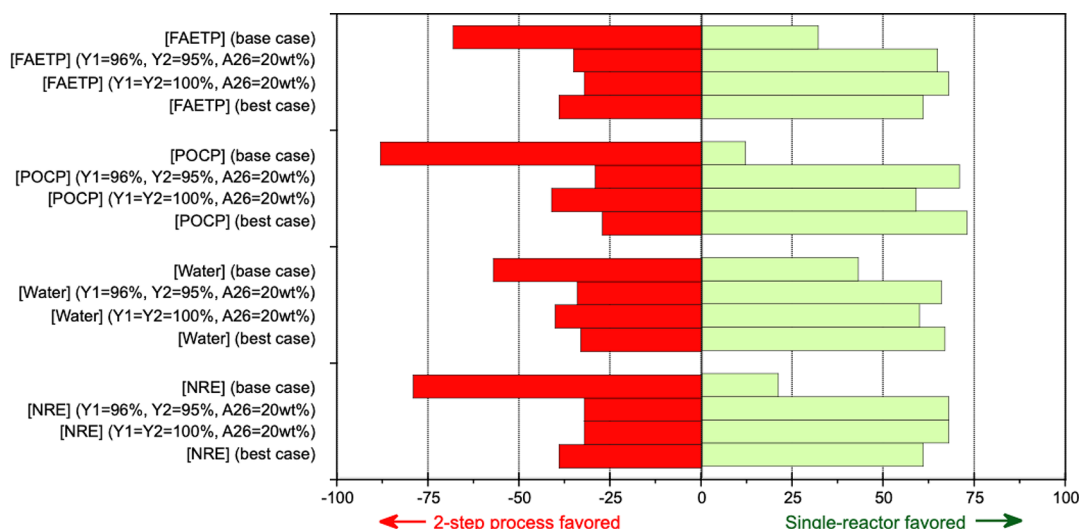


Figure 20. Uncertainty analysis for two-reactor and single-reactor processes issued from MC analysis unveil the statistical significance of the values measured for the following impact categories: [NRE], [Water], [POCP], and [FAETP] ($C = 3$). The following scenarios were considered: (1) base case 1 for both processes; (2) $Y1 = 96\%$, $Y2 = 95\%$, and $A26 = 20\text{ wt } \%$ (base case 1 for a two-step process and base case 2 for a single-reactor process); (3) $Y1 = Y2 = 100\%$, $A26 = 20\text{ wt } \%$; and (4) best case for both processes.

processes; log-normal plots from MC analysis for [NRE], [Water], [POCP], and [FAETP]; physicochemical properties of chemicals for F-ALD-1-NH₂ production; process inventory for F-ALD-1-NH₂ production; summary of process assumptions; Ru inventory in Ecoinvent 3.4; amount of Ru reused and cost as a function of the number of regeneration cycles (C) of the Ru/C catalyst; pedigree matrix and scores for both processes; scores used for the pedigree matrix; breakdown of fixed and variable (base case) costs; sensitivity analysis for FMC for both processes; breakdown of NRE for both processes; sensitivity analysis for the different impact categories for both processes; definition of environmental impacts (DOCX)

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Notes

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GLOSSARY VARIABLES

C	number of regeneration cycles of the Ru/C catalyst (-)
CF	characterization factor of substance i in eq 1 (variable unit)
impact _{j}	impact attributed to variable j in eq 1 (variable unit)
IRR	internal return rate (%)
m_i	emission of substance i (-)
MSP	minimum selling price (€)
R1	MIBK/FF molar ratio (-)
R2	EtOH/FF molar ratio (-)

GREEK SYMBOLS

σ uncertainty factor (-)

ACRONYMS

A26	Amberlyst A26
[AP]	acidification potential
[ADP]	abiotic depletion potential
ALD-1	(<i>E</i>)-1-(furan-2-yl)-5-methylhex-1-en-3-one
CAPEX	capital expenditure
CML	Centrum voor Milieukunde Leiden
[EP]	eutrophication potential
EtOH	ethanol
FF	furfural
FMC	full manufacturing cost
GLO	global market dataset
F-ALD-1	1-(furan-2-yl)-5-methylhexan-3-one
F-ALD-1-NH ₂	1-(furan-2-yl)-4-methylpentan-2-amine
[FAETP]	freshwater aquatic ecotoxicity potential
[GWP 100a]	global warming potential
[HTP]	human toxicity potential
IPA	International Platinum Group Metal Association
ISBL	inside battery limits
[Land Use]	quantitative land use
LCI	life cycle inventory
LCIA	life cycle impact assessment

LCA	life cycle assessment
[MAETP]	marine aquatic ecotoxicity potential
MIBK	methyl isobutyl ketone
MC	Monte Carlo
[NRE]	nonrenewable energy
[OLDP]	ozone layer depletion potential
OPEX	operational expenditure
OSBL	outside battery limits
PGM	platinum group metals
[Renew]	renewable energy
RER	European Regional
[POCP]	photochemical oxidant creation potential
SPM	Solvay Portfolio Management
TEA	technoeconomic assessment
[TETP]	terrestrial ecotoxicity potential
THF-ALD-1	5-methyl-1-(tetrahydrofuran-2-yl)hexan-3-one
[Water]	water use

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