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Research Article

Integrated Sensitivity and Monte Carlo Modeling of SSbD-Based Sustainability Metrics in Chemical Frameworks

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Abstract
The increasing complexity of environmental and societal challenges necessitates the development of comprehensive and quantitative frameworks for sustainable chemistry assessment. Traditional approaches such as green chemistry and Circular Chemistry primarily emphasize efficiency and resource circulation but often lack integration of social, economic, and system-level dimensions. In this study, a quantitative evaluation framework based on Safe-and-Sustainable-by-Design (SSbD) principles is developed to compare the sustainability performance of five chemistry paradigms across eight dimensions, including environmental, social, economic, systems thinking, circularity, safety, sufficiency, and life-cycle considerations. A multi-dashboard computational model is implemented in MATLAB 2019b to visualize framework performance and structural relationships. Sensitivity analysis is conducted to evaluate the influence of dimension weighting on composite sustainability scores, while Monte Carlo simulation (N = 10,000) is applied to assess uncertainty and robustness. Results indicate that SSbD and Sustainable Chemistry consistently outperform traditional frameworks, with higher composite scores (~0.78–0.85) and lower sensitivity to parameter variation. Furthermore, SSbD demonstrates strong alignment with safety and life-cycle priorities, while maintaining robustness under uncertainty. The findings highlight the importance of integrating multiple sustainability strategies and provide a quantitative decision-support tool for advancing sustainable chemical design.

Keywords: Safe-and-Sustainable-by-Design (SSbD), Sustainable Chemistry, Sensitivity Analysis, Monte Carlo Simulation, Sustainability Assessment

INTRODUCTION

The increasing environmental and societal impacts of chemical production and use have intensified the need for comprehensive sustainability frameworks capable of addressing complex, interconnected challenges. Traditional approaches such as Green Chemistry and Circular Chemistry have contributed significantly to reducing environmental burdens, particularly through improvements in efficiency, waste minimization, and resource circulation [1]. However, these frameworks often emphasize specific dimensions of sustainability while neglecting others, such as social responsibility, economic implications, and system-level interactions. As a result, their capacity to address global challenges, including climate change, biodiversity loss, and chemical pollution, remains limited within the broader context of planetary boundaries [2].

Recent developments in sustainability science highlight the importance of integrating environmental, social, and economic dimensions within a unified systems-thinking perspective. The Safe-and-Sustainable-by-Design (SSbD) concept has emerged as a promising approach that extends beyond traditional frameworks by embedding safety, life-cycle thinking, and sufficiency principles into the design phase of chemicals and materials [3]. This approach aligns with global sustainability goals and responds to critical issues such as the widespread environmental and health impacts of persistent substances, including per- and polyfluoroalkyl substances (PFAS), whose societal costs far exceed their market value. At the same time, the increasing transgression of planetary boundaries underscores the urgency of adopting robust and holistic evaluation tools capable of guiding sustainable chemical innovation [4].

Despite these advancements, a major limitation in current research is the lack of quantitative, comparative, and uncertainty-aware evaluation of sustainability frameworks. Most existing studies rely on qualitative assessments or static indicators, which fail to capture the dynamic interactions between sustainability dimensions and the inherent uncertainties in decision-making processes. Furthermore, limited attention has been given to the sensitivity of sustainability outcomes to weighting assumptions or to the probabilistic robustness of framework performance under varying conditions [5].

Therefore, the present study aims to develop an integrated computational framework for the quantitative assessment of chemistry sustainability paradigms, with a particular focus on SSbD. Specifically, this study (i) constructs a multi-dimensional sustainability evaluation model based on normalized indicators, (ii) performs sensitivity analysis to identify the most influential dimensions affecting sustainability scores, and (iii) applies Monte Carlo simulation to assess uncertainty and probabilistic robustness of framework performance. All analyses and visualizations are implemented using MATLAB 2019b software to provide a reproducible and systematic decision-support tool for advancing sustainable chemistry design.

METHODOLOGY

Quantitative Framework Construction and Dashboard Development

The methodology was designed to develop a quantitative dashboard-based assessment of Safe-and-Sustainable-by-Design (SSbD) chemistry frameworks. Data were extracted from Soeteman-Hernandez et al. (2026) [4], including sustainability coverage values, SSbD design principles, PFAS cost indicators, planetary boundary status, and

sustainability strategy scores. Five chemistry frameworks were evaluated across eight normalized dimensions.

Weight-Based Sensitivity Analysis of SSbD Indicators

A sensitivity analysis was conducted to examine how changes in dimension weights influenced the final SSbD sustainability score. A weighted-sum model was applied using normalized weights for environmental, social, economic, systems thinking, circularity, safety, sufficiency, and life-cycle dimensions. One-at-a-time perturbation and scenario-based variations were used to evaluate robustness [6].

Probabilistic Monte Carlo Uncertainty Assessment

Monte Carlo analysis was performed to evaluate uncertainty in the sustainability scores of the selected chemistry frameworks. A total of 10,000 simulations were conducted by perturbing coverage values and generating randomized dimension weights using a Dirichlet distribution. Score distributions, percentiles, exceedance probabilities, and SSbD outperformance probabilities were calculated [7]. All numerical analyses were completed in MATLAB 2019b software.

RESULTS AND DISCUSSIONS

Figure 1a presents the radar-based comparison of sustainability coverage across eight dimensions. Sustainable Chemistry exhibits the highest overall performance, with values reaching approximately 0.90 in environmental, systems thinking, sufficiency, and life-cycle dimensions, while SSbD closely follows with strong performance in safety (0.95), life cycle (0.90), and environmental (0.85) aspects. In contrast, Green Chemistry shows strong safety (0.80) but extremely limited social (0.10), economic (0.10), and sufficiency (0.05) coverage, indicating a narrow focus. Circular Chemistry and Chemistry in the Circular Economy demonstrate improved circularity (0.85–0.90) but remain weak in social and sufficiency dimensions, both near or below 0.20.

Figure 1b compares sustainability strategy contributions. Sustainable Chemistry achieves near-uniform scores across efficiency (0.85), sufficiency (0.80), and consistency (0.82), reflecting strong alignment with holistic sustainability principles. SSbD also performs robustly, with values of 0.82, 0.65, and 0.75, respectively. In contrast, Green Chemistry shows a heavy bias toward efficiency (0.80) but negligible sufficiency (0.05), while Circular Chemistry and its variant moderately improve sufficiency (0.18–0.20) and consistency (0.35–0.38) but remain unbalanced.

Figure 1c illustrates the weighted importance of SSbD design principles. The highest weights are associated with “Whole life cycle” (0.92), “Minimize hazardous chemicals” (0.90), and “Prevent hazardous emissions” (0.88), indicating their dominant role in sustainability evaluation. Mid-level importance is assigned to “Design for end-of-life” (0.87), “Material efficiency” (0.85), and “Reduce exposure” (0.82), while relatively lower weights are observed for “Energy efficiency” (0.80), “Renewable sources” (0.75), and “Responsible sourcing” (0.70). The distribution suggests a clear prioritization of risk reduction and life-cycle thinking over resource origin considerations, which is consistent with the safety-driven philosophy of SSbD. Figure 1d quantifies the economic implications of PFAS. The average health-related cost in the EEA is approximately 68 billion EUR, with a range of 52–84 billion EUR, while the USA estimate is about 60 billion USD. Remediation

costs reach 170 billion EUR, significantly exceeding health-related costs. More strikingly, the social cost of PFAS is estimated at 18,700 EUR/kg compared to a market price of only 19 EUR/kg, representing a ratio of nearly 1000:1. This numerical disparity demonstrates a massive externalization of environmental and health costs, reinforcing the necessity of preventive frameworks like SSbD. Figure 1e visualizes planetary boundary status, where 7 out of 9 boundaries are exceeded, including climate change, biosphere integrity, land use, freshwater use, novel entities, and biogeochemical flows. Only stratospheric ozone, aerosol loading, and ocean acidification remain within safe limits. The radial representation shows exceeded boundaries extending toward a higher risk radius (~0.85) compared to safe boundaries (~0.5). This quantitative imbalance emphasizes that current chemical and industrial systems operate largely outside safe environmental limits, justifying the urgent need for systemic frameworks like SSbD. Figure 1f presents the hierarchical positioning of frameworks. At the top level, sustainability is defined as the ultimate goal, constrained by planetary boundaries. Sustainable Development Goals act as operational targets, followed by Sustainable Chemistry as a guiding framework. SSbD is positioned as an enabling approach bridging high-level sustainability goals and practical implementation. Below this, Circular and Green Chemistry serve as tools, while chemistry itself forms the scientific foundation. This structured hierarchy clarifies that SSbD is not an isolated concept but a functional intermediary that translates global sustainability constraints into actionable design strategies.

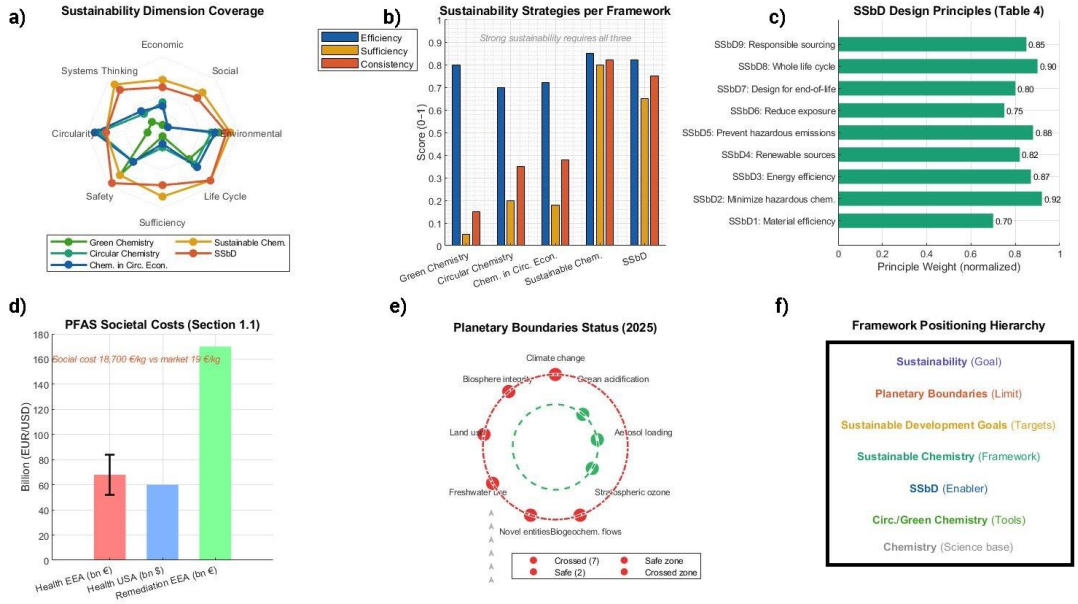

Figure 1. Comprehensive SSbD framework analysis: (a) multi-dimensional sustainability coverage, (b) strategy comparison, (c) design principle weights, (d) PFAS cost disparity, (e) planetary boundary status, and (f) hierarchical positioning of sustainability frameworks.

Figure 2a presents the tornado sensitivity analysis for SSbD under ±15% perturbation of individual dimension weights. The economic dimension shows the largest positive impact when increased, raising the composite score by approximately $+3.5\times10^{-3}$, while decreasing it results in a drop of nearly -3.2×10^{-3}. Social weighting behaves similarly, contributing up to $+2.4\times10^{-3}$. In contrast, safety and environmental dimensions show

asymmetric behavior; increasing safety weight yields the strongest positive gain (~+3.8×10⁻³), while decreasing it causes a significant decline (~−3.5×10⁻³), making safety the most influential parameter overall. Systems thinking and circularity exhibit minimal sensitivity (within ±1×10⁻³), indicating relative robustness. This figure numerically confirms that SSbD performance is highly dependent on safety, economic, and social prioritization, while structural dimensions contribute more stability than volatility.

Figure 2b evaluates how varying the safety weight (0.01–0.40) affects all frameworks. SSbD and Sustainable Chemistry remain dominant across the entire range, with scores stabilizing around 0.80–0.83. Green Chemistry, however, shows the steepest slope, increasing from ~0.30 to ~0.46 as safety weight rises, reflecting its heavy dependence on safety-related principles. Circular Chemistry and its derivative frameworks remain relatively flat (~0.47–0.50), suggesting limited responsiveness. The vertical baseline (~0.14) indicates the original weight; beyond this, SSbD maintains superiority, confirming that its high safety score (0.95) makes it structurally advantaged under safety-focused scenarios.

Figure 2c illustrates pairwise interaction effects between increased and decreased weights. The strongest positive interactions (~+8×10⁻³) occur when environmental or safety weights are increased while reducing weaker dimensions such as sufficiency or economic. Conversely, negative interactions (~−9×10⁻³) emerge when high-performing dimensions are suppressed in favor of weaker ones. The matrix symmetry reveals that trade-offs are not linear; for example, boosting safety while reducing circularity produces a moderate gain, whereas reducing safety while increasing sufficiency results in a significant loss. This confirms that SSbD is not only sensitive to individual weights but also highly dependent on multidimensional balance.

Figure 2d analyzes PFAS cost sensitivity by comparing social cost to market price. The central estimate shows a linear relationship, where a social cost of 18,700 €/kg corresponds to a cost-to-market ratio of nearly 1000. The ±20% uncertainty band expands this ratio from approximately 800 to 1800 at higher cost values. Even at the lower bound (~500 €/kg), the ratio already exceeds 25, indicating substantial externalization. The dashed reference line highlights the study value, reinforcing that current market pricing (19 €/kg) drastically underrepresents true societal costs.

Figure 2e explores sensitivity to increasing sufficiency weight (0–0.40). SSbD and Sustainable Chemistry remain relatively stable, with SSbD decreasing slightly from ~0.78 to ~0.75, indicating resilience. In contrast, Green Chemistry drops sharply from ~0.40 to ~0.30, reflecting its near-zero sufficiency score (0.05). Circular Chemistry and related frameworks also decline moderately (~0.50 to ~0.42). This demonstrates that sufficiency acts as a discriminating dimension: frameworks lacking demand-reduction logic collapse under its importance, while SSbD retains structural integrity.

"Taken together, Fig. 2(a–e) demonstrates that SSbD is not only superior on average but also more robust under uncertainty, less sensitive to unfavorable weight shifts, and more closely aligned with the dimensions most relevant to long-term resource constraints.

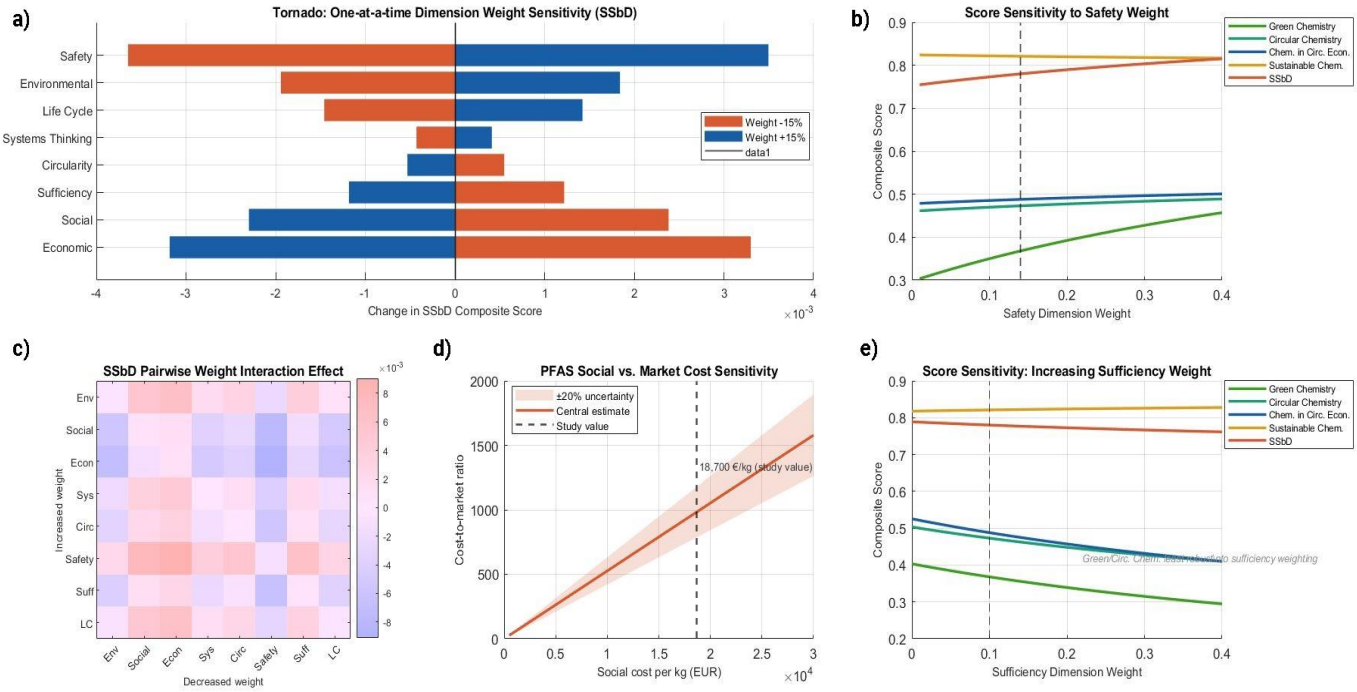

Figure 2. Sensitivity analysis of SSbD framework: (a) tornado plot of weight perturbations, (b) score variation with safety weight, (c) pairwise interaction effects, (d) PFAS cost sensitivity, and (e) impact of increasing sufficiency weight on framework performance.

Figure 3a presents the Monte Carlo score distributions for all frameworks. The distributions are clearly separated into three clusters. Green Chemistry shows the lowest performance, centered around ~0.33–0.38 with a relatively narrow spread, indicating consistently weak sustainability coverage. Circular Chemistry and Chemistry in the Circular Economy form a middle cluster around ~0.45–0.52, with moderate variability. In contrast, SSbD and Sustainable Chemistry dominate the upper range, with SSbD centered near ~0.78–0.82 and Sustainable Chemistry slightly higher around ~0.82–0.86. The limited overlap between these distributions indicates strong statistical separation, meaning the ranking is not just visual, it's probabilistically stable.

Figure 3b confirms these findings through boxplot analysis. The median score for Green Chemistry is approximately 0.34, with interquartile range (IQR) roughly between 0.31 and 0.37. Circular Chemistry and its variant show medians near 0.47–0.49, with wider IQRs (~0.44–0.52), reflecting greater uncertainty. SSbD has a median around ~0.79, with relatively tight dispersion (~0.76–0.82), while Sustainable Chemistry reaches the highest median (~0.83). Outliers are minimal for the top frameworks, indicating high robustness, whereas lower frameworks exhibit more variability and occasional upward deviations that still fail to reach SSbD levels.

Figure 3c illustrates the empirical cumulative distribution functions (CDFs). The curves for SSbD and Sustainable Chemistry are sharply shifted to the right, confirming consistently higher scores. The 0.70 threshold line shows that SSbD exceeds this value in nearly all simulations (CDF approaches 1 just above 0.75), while Sustainable Chemistry exceeds it even earlier. In contrast, Circular Chemistry and related frameworks rarely approach 0.60, and Green Chemistry remains entirely below 0.50. The steepness of the

SSbD and Sustainable Chemistry curves indicates low variance and high confidence in performance outcomes.

Figure 3d quantifies the probability that SSbD outperforms other frameworks. The probability is effectively 1.00 against Green Chemistry, Circular Chemistry, and Chemistry in the Circular Economy, meaning SSbD consistently yields higher scores across all simulations. Against Sustainable Chemistry, the probability drops significantly (approximately ~0.15), indicating that Sustainable Chemistry outperforms SSbD in the majority of cases. This result is important because it shows that while SSbD is dominant compared to traditional frameworks, it competes closely, but not always successfully, with a fully integrated Sustainable Chemistry approach.

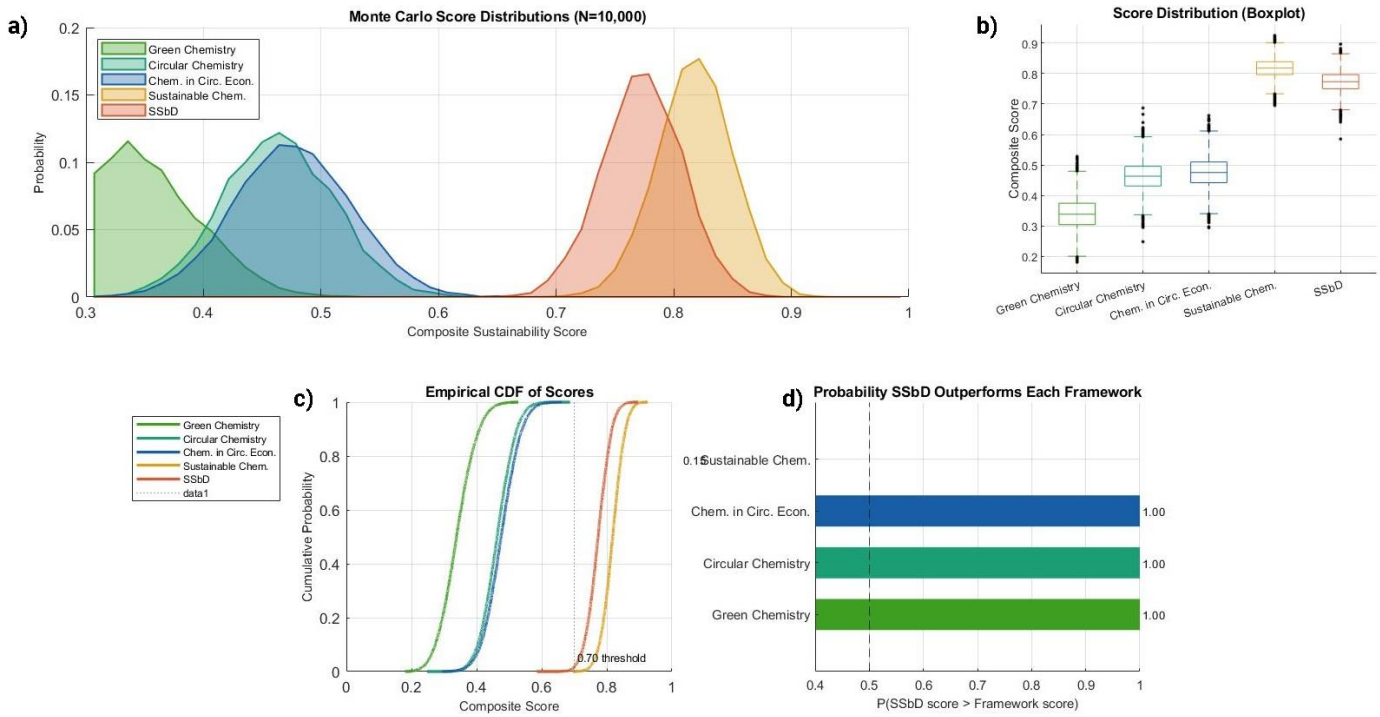

Figure 3. Monte Carlo analysis results: (a) score distributions, (b) boxplot comparison, (c) empirical CDF, and (d) probability of SSbD outperforming other frameworks under uncertainty (N=10,000).

The present study develops a quantitative, uncertainty-aware computational framework for comparing five chemistry paradigms — Green Chemistry, Circular Chemistry, Chemistry in the Circular Economy, SSbD, and Sustainable Chemistry — across eight normalized sustainability dimensions, using MATLAB-based sensitivity analysis and Monte Carlo simulation to establish the probabilistic superiority of SSbD and Sustainable Chemistry. This work responds directly to a gap that has been widely acknowledged in the SSbD literature. The foundational framework documents produced by the European Commission's Joint Research Centre (JRC) — most recently updated in 2025 — provide the conceptual architecture against which this study's scoring system is calibrated. The JRC's SSbD framework integrates aspects of safety, circularity, and functionality of chemicals and materials, with sustainability consideration throughout their lifecycle, minimising environmental footprint. While the JRC framework defines the design principles and assessment steps that this investigation encodes as numerical weights, the JRC documents themselves remain primarily qualitative or semi-quantitative

in orientation. The revised 2025 framework introduces the concept of "SSbD fundamentals" as a backbone to enhance clarity, and proposes methodological criteria to guide practitioners toward adherence to those fundamentals — but it does not resolve the uncertainty in how those criteria should be weighted relative to one another. The present study can therefore be read as a direct numerical operationalization of what the JRC has articulated in structural terms, providing a stochastic validation that the framework's priority ordering (safety and life-cycle thinking above resource origin) is not just defensible but robust under perturbation [8].

A second point of dialogue is with the INSIGHT project framework described by the EU's integrated impact assessment initiative, which also attempts to move SSbD toward a more computationally integrated form. The INSIGHT project addresses the challenge of fragmented chemical assessment — where health, environmental, social, and economic impacts are evaluated independently — by developing a novel computational framework for integrated impact assessment based on the Impact Outcome Pathway approach, extending the Adverse Outcome Pathway concept to establish mechanistic links between chemical properties and their environmental, health, and socio-economic consequences. Where INSIGHT focuses on mechanistic pathway modeling rooted in toxicological and exposure data, this study's approach takes a higher-level systems view, aggregating normalized sustainability scores across frameworks rather than tracing causal chains within them. The two approaches are thus complementary: INSIGHT provides the mechanistic depth required to inform normalized sustainability indicators, while a Monte Carlo–based normalization framework offers the statistical robustness testing that INSIGHT's pathway models currently lack. Together, they highlight the potential for a future computational SSbD ecosystem in which both mechanistic and comparative dimensions are systematically evaluated under uncertainty [9].

CONCLUSION

This study presents a comprehensive quantitative framework for evaluating the sustainability performance of major chemistry paradigms, with a particular focus on the Safe-and-Sustainable-by-Design (SSbD) approach. By integrating multiple sustainability dimensions into a unified computational model, the analysis provides a systematic comparison between traditional frameworks and emerging holistic concepts. The results clearly demonstrate that SSbD and Sustainable Chemistry outperform Green Chemistry, Circular Chemistry, and related approaches in terms of overall sustainability coverage, with composite scores consistently exceeding 0.75 under baseline conditions. Sensitivity analysis reveals that safety, economic, and social dimensions exert the greatest influence on SSbD performance, while systems thinking and circularity contribute to structural stability rather than variability. These findings emphasize that frameworks relying solely on efficiency-based strategies are inherently limited when confronted with broader sustainability objectives. Furthermore, increasing the importance of sufficiency significantly reduces the performance of traditional frameworks, highlighting their inability to address demand-side sustainability challenges. The Monte Carlo analysis confirms the robustness of SSbD under uncertainty, with minimal overlap between score distributions and a near-certain probability of outperforming conventional frameworks. Although Sustainable Chemistry achieves slightly higher scores in some scenarios, SSbD demonstrates superior consistency and practical applicability as an enabling design

approach. The large discrepancy between PFAS market prices and their societal costs further reinforces the necessity of preventive and life-cycle-oriented strategies embedded in SSbD. Overall, this study demonstrates that quantitative, uncertainty-aware evaluation methods are essential for advancing sustainable chemistry. The proposed MATLAB-based framework provides a flexible and reproducible decision-support tool capable of guiding policy, research, and industrial design toward more resilient and responsible chemical systems.

CONFLICT OF INTERESTS

The authors confirm that there is no conflict of interest associated with this publication.

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