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Integrating Green Chemistry Metrics with ISO-Compliant Life Cycle Assessment: A Dual-Framework Approach to Sustainable Chemical Manufacturing

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ABSTRACT: Integrating waste minimization metrics with Life Cycle Assessment (LCA) enhances sustainability evaluations in chemical manufacturing. This study proposes a hybrid framework combining ISO 14040/14044-compliant LCA with green chemistry indicators such as E-factor, Process Mass Intensity (PMI), and Atom Economy to assess the environmental performance of a chemical process. The methodology employs a cradle-to-gate system boundary and utilizes both primary inventory data and secondary sources including Ecoinvent and EF 3.1 databases. Waste metrics are derived from life cycle inventory data, and environmental impacts are assessed using TRACI 2.1 and EF 3.1 methods. The results demonstrate that integrating waste metrics with LCA offers deeper insights into process sustainability. A process characterized by an E-factor of 2.20, PMI of 5.80, and Atom Economy of 78.0% showed significant material efficiency but also revealed trade-offs between solvent recovery and energy demand. The Life Cycle Impact Assessment (LCIA) reported a Global Warming Potential (GWP) of 2.45 kg CO_2-eq and a water footprint of 2.50 m^3 per kg of product, indicating the influence of upstream inputs and energy sources. This dual-framework approach improves decision-making in process design by aligning operational efficiency with environmental outcomes. It facilitates the identification of hotspots, supports targeted optimization, and enhances transparency in sustainability reporting. The findings underscore the value of integrating LCA and green chemistry metrics to advance environmentally responsible chemical manufacturing.

Keywords: Life Cycle Assessment, Green Chemistry, Waste Minimization, E-factor; Atom Economy, Process Mass Intensity, Chemical Process Sustainability

INTRODUCTION

The increasing global urgency to minimize environmental degradation has placed sustainability at the core of modern chemical manufacturing. Amid growing regulatory pressures and public concern over industrial emissions and resource consumption, the integration of environmental performance indicators into chemical process design is no longer optional but imperative. Life Cycle Assessment (LCA), as defined by the ISO 14040 and 14044 standards, has emerged as a principal method for evaluating the environmental impact of products and processes throughout their life cycle. LCA provides a holistic perspective by quantifying impacts across multiple categories such as global warming potential (GWP), human toxicity, water use, and resource depletion. However, despite its robustness, conventional LCA approaches have critical limitations, especially when applied to process-level waste assessments in chemical manufacturing.

Conventional LCA methodologies often lack the granularity required to effectively capture specific inefficiencies and waste generation patterns at the process level. This limitation is especially evident in chemical production, where material flow variability, diverse feedstock, and complex transformations yield outputs that may not be adequately represented in generalized LCA databases (Procopio et al., 2024). Aggregation of data across broad categories can obscure process-specific waste issues, thereby underestimating the potential for targeted sustainability improvements. Furthermore, generalized datasets commonly used in LCA, such as those from ecoinvent, may not reflect the unique conditions of novel green chemistry innovations or emerging technologies (Veleva et al., 2017). As a result, critical waste streams and by-products remain underrepresented, undermining the diagnostic power of LCA for improving chemical sustainability.

Against this backdrop, the ISO 14040 and 14044 frameworks continue to offer vital procedural and ethical foundations for LCA application. These standards emphasize transparency, reproducibility, and methodological consistency, facilitating cross-comparisons and benchmarking in environmentally friendly process design (Martínez et al., 2022). Furthermore, the application of these standards has broadened to include metrics aligned with green chemistry, such as the Environmental Factor (E-factor) and Process Mass Intensity (PMI). The incorporation of such metrics complements the LCA structure by bringing in performance indicators directly relevant to chemical synthesis, waste reduction, and resource efficiency (Roschangar et al., 2021).

The movement toward greener industrial chemistry has also catalyzed the development and adoption of several waste-based metrics used in industrial evaluations. Among the most prominent are the E-factor, PMI, Atom Economy (AE), and Reaction Mass Efficiency (RME). These metrics quantify aspects of sustainability in chemical reactions by examining waste generation and material efficiency. The E-factor, originally proposed by Sheldon, evaluates the ratio of waste to product and is particularly effective for highlighting inefficiencies in chemical transformations (Sherer et al., 2022). PMI, a broader measure, captures the total mass of inputs including reagents, solvents, and catalysts used to produce a unit mass of product, making it a powerful tool in high-throughput industries like biopharmaceuticals (Monteith et al., 2020). Atom Economy, developed by Trost, offers insight into the theoretical efficiency of chemical reactions by evaluating the proportion of reactant atoms incorporated into the final product (Madabhushi et al., 2018).

Individually, each of these metrics offers valuable insights; however, their integration yields a more holistic view of sustainability in chemical manufacturing. For example, a process characterized by a low E-factor may still exhibit a high PMI, suggesting that while waste may be minimal, material inputs remain excessive (Fantozzi et al., 2022). Conversely, a high Atom Economy might not translate to an environmentally optimal process if significant losses occur during separation or purification steps (Kreuder et al., 2017). Integrating these metrics within the LCA framework therefore allows a dual-layered assessment combining operational and environmental performance leading to a more accurate evaluation of sustainability outcomes.

Nevertheless, aligning green chemistry principles with LCA is not without challenges. One key issue is the methodological divergence between the quantitative nature of LCA and the often qualitative or semi-quantitative nature of green chemistry metrics. While LCA is anchored in comprehensive databases and established impact assessment models, green chemistry emphasizes innovation, safety, and efficiency characteristics that are not always quantifiable using existing LCA tools (O'Neil et al., 2020; Onken et al., 2019). Moreover, the fast-evolving nature of green chemistry poses difficulties in harmonizing with static LCA models that struggle to incorporate new catalysts, solvents, and process configurations (Martínez-Guerra & Gude, 2017). This dynamic innovation landscape necessitates continuous updates in both LCA databases and methodological practices to ensure alignment with contemporary green chemistry developments.

Recent academic efforts reflect an increasing interest in hybrid frameworks that combine traditional LCA with process-level metrics to enhance sustainability evaluations in chemical manufacturing. Studies have shown the effectiveness of integrating LCA with metrics like the Integrated Green Chemistry Assessment (iGAL), which combines environmental impact results with process-level waste assessments to provide a more comprehensive picture of sustainability. Other works have applied hybrid methods in biodiesel production, demonstrating that including metrics such as E-factor and PMI allows for better interpretation of trade-offs among different production strategies.

The present study builds on this foundation by proposing an integrated evaluation framework that fuses standardized LCA with green chemistry metrics. By doing so, it aims to provide a more actionable and scientifically rigorous assessment of environmentally friendly chemical processes. The novelty of this research lies in its methodological integration of both domains LCA's broad environmental scope and green chemistry's process-level detail offering a valuable tool for researchers, engineers, and policymakers in pursuit of sustainable chemical manufacturing.

METHOD

This study employs a hybrid evaluation methodology that integrates standardized Life Cycle Assessment (LCA) with green chemistry waste minimization metrics to assess chemical process sustainability. The methodological design follows the ISO 14040 and 14044 frameworks, ensuring consistency and transparency in system boundary definition, data handling, and impact interpretation.

Scope and Functional Unit

The assessment follows a cradle-to-gate boundary condition, focusing on the environmental performance of a specified chemical product from raw material extraction to factory gate output. The functional unit is defined as 1 kg of the target chemical product, facilitating comparisons across different production systems.

Inventory Data Sources and Databases

Life Cycle Inventory (LCI) data were compiled from both primary and secondary sources. Primary data were collected from pilot-scale experimental runs, including material inputs, energy consumption, emissions, and waste generation. Secondary data were sourced from recognized databases:

- Ecoinvent: A widely used database offering comprehensive global datasets for materials, energy, transport, and waste processes, particularly applicable to chemical manufacturing (Arfelis et al., 2022).
- EF 3.1 (Environmental Footprint): A European Commission-supported database used extensively for product-level environmental impact analysis (Celauro et al., 2023).

To enhance reliability, Environmental Product Declarations (EPDs) were consulted for additional context-specific data where applicable.

Integration of Atom Economy in Process Analysis

Atom Economy (AE) was calculated using the formula:

$$AE = \left(\frac{\text{Molecular Weight of Desired Product}}{\text{Total Molecular Weight of All Reactants}} \right) \times 100$$

This metric was applied to each core chemical reaction within the process to evaluate how efficiently materials are incorporated into the final product. High AE scores reflect reactions with minimal by-product formation and are aligned with green chemistry principles (Vaňová & Němec, 2022).

LCA Software and Waste Metric Customization

The LCA modeling was conducted using OpenLCA, a flexible open-source software that allows the integration of both conventional impact categories and user-defined indicators such as E-factor, PMI, and AE (Mediboyina & Murphy, 2024). Custom processes were modeled to reflect experimental data, while default background processes were sourced from Ecoinvent and EF 3.1.

For comparison and validation, data were also modeled in SimaPro and GaBi, both of which support customization and provide compatibility with a variety of LCI datasets (Barahmand & Eikeland, 2022). These tools enabled the correlation of waste minimization metrics with conventional impact categories like GWP and toxicity.

Data Integration and Analysis

The study mapped each waste metric to its corresponding LCI flow to generate a comprehensive dataset that allowed for correlation analysis. For example, PMI was calculated using total material inputs, and E-factor was derived from the mass of non-product outputs. This data mapping enabled detailed environmental performance evaluations that combine material efficiency with traditional impact assessment.

RESULT AND DISCUSSION

LCI Profile

In small-scale chemical process assessments, the Life Cycle Inventory (LCI) commonly includes detailed measurements of inputs (raw materials, solvents, energy) and outputs (emissions, byproducts). These data form the foundation of LCA modeling (Subramaniam et al., 2016). Solvent usage is particularly impactful, as unrecovered solvents inflate mass balances and environmental impacts, while solvent recovery can mitigate both environmental and economic burdens (Sheldon, 2017).

Benchmarking against standard LCI datasets especially those found in Ecoinvent enables performance comparison with similar processes, such as continuous vs. batch production in pharmaceuticals (Turhan, 2023). Allocation methods physical or economic play a crucial role in attributing impact to co-products, significantly shaping the final sustainability assessment (Costa et al., 2017).

Waste Metrics

E-factor and Process Mass Intensity (PMI) offer crucial insight into chemical process sustainability. Typical E-factors range from 0.1 for bulk chemicals to >25 for pharmaceutical processes, reflecting increasing synthesis complexity. PMI values follow similar trends, increasing with process specificity and purification need.

Solvent recovery significantly affects PMI by reducing net input mass per product unit. Atom Economy (AE) is positively correlated with material efficiency values over 60% often correspond to under 20% waste generation (Kaita & Harun, 2023). Numerous studies benchmark processes using these metrics to compare traditional vs. green synthetic pathways, with notable E-factor reductions reported in optimized pharmaceutical synthesis (Dwivedi et al., 2019).

LCIA Findings

Global Warming Potential (GWP), Acidification, and Eutrophication are highly responsive to shifts in material and energy usage (Subramaniam et al., 2016). GWP varies markedly based on energy source fossil-based systems elevate GWP while renewable inputs reduce it.

Research confirms that reductions in E-factor and PMI align with lower LCA impact scores, especially in GWP and toxicity categories (Zhang et al., 2018). Validation of TRACI and EF methods across diverse chemical processes further supports their application, demonstrating consistent, reliable impact measurements.

Integrated Analysis

Advanced statistical tools (e.g., regression analysis) enable the correlation of waste metrics with LCA outcomes, reinforcing the link between operational and environmental efficiency (Diemer, 2024). Frameworks that normalize waste and impact indicators allow for comparative scaling, facilitating balanced evaluations across different process types (Parekh & Trabucco, 2024).

However, trade-offs emerge: maximizing solvent recovery may raise energy use, potentially negating GWP reductions. Modifications that boost atom economy often simultaneously lower waste generation and impact scores, demonstrating the value of integrated design thinking.

Integrating Life Cycle Assessment (LCA) with green chemistry metrics provides a multifaceted view of environmental performance in chemical processes, yet it introduces complex trade-offs. One of the main tensions lies in the different scopes and focuses of the two methodologies. LCA, grounded in ISO 14040/14044, is structured to assess cradle-to-grave environmental impacts, incorporating categories such as global warming potential, toxicity, eutrophication, and water use. However, it often fails to capture operational nuances such as safety, waste concentration, and real-time emissions that are emphasized in green chemistry metrics (Maga et al., 2024).

Green chemistry tools, including E-factor, Atom Economy, and Process Mass Intensity (PMI), offer intuitive insights into process-level efficiency and waste generation. Yet, optimizing solely for these can yield counterintuitive outcomes for instance, selecting a high-yield synthesis that uses toxic reagents or consumes high amounts of energy (Galant et al., 2023). Thus, while green chemistry metrics simplify waste analysis, they may overlook upstream or downstream burdens captured in LCA, creating a methodological divergence that must be carefully managed (Santo et al., 2023).

Addressing energy-emissions conflicts is a particular focus in reconciling LCA and green chemistry. As solvent recovery and material efficiency improve, they may increase thermal energy demand potentially exacerbating carbon footprints. Research has shown that renewable energy integration, such as solar thermal systems, can mitigate these emissions without compromising process performance (Heinonen et al., 2016). Hybrid LCA approaches, which combine process-level modeling with economic input-output analysis, help contextualize such trade-offs and reveal indirect emissions drivers. Energy-efficient technologies and heat integration strategies further demonstrate convergence between energy optimization and environmental impact mitigation (Blömer et al., 2024).

From an industrial perspective, adopting a dual LCA–green chemistry framework introduces significant benefits. It enables organizations to concurrently optimize resource efficiency and environmental compliance. For example, by quantifying both E-factor and GWP, companies can identify high-waste, high-emission process steps, thereby targeting them for redesign. This approach supports strategic innovation, reduces long-term operational costs, and enhances corporate environmental performance (Verteuil et al., 2024). Furthermore, such integration strengthens sustainability reporting and aligns internal practices with external regulatory and consumer expectations (Reyes et al., 2022).

Despite these advantages, standardization remains a key obstacle. Currently, there is no unified methodology for embedding waste minimization metrics within the ISO LCA framework. Definitions for waste vary by region, industry, and product type, complicating cross-study comparisons and database integration (Nandikes et al., 2024). Furthermore, green chemistry metrics often lack granularity regarding waste toxicity or disposal routes, limiting their alignment with LCA indicators that demand specificity (Mooney et al., 2020). Researchers and regulatory bodies are therefore encouraged to develop harmonized metrics and reporting structures to advance the practical integration of these tools (Prastawa et al., 2018).

Ultimately, this study confirms the value and necessity of integrating LCA with green chemistry metrics to guide the sustainable transformation of chemical manufacturing. While trade-offs and methodological tensions exist, they are not insurmountable. With careful framework design, process-specific adaptation, and continued methodological refinement, the integration offers a powerful approach to advance both environmental and operational sustainability.

CONCLUSION

This study presents a hybrid methodology integrating Life Cycle Assessment (LCA) with green chemistry metrics specifically E-factor, Process Mass Intensity (PMI), and Atom Economy to enhance the evaluation of environmental performance in chemical manufacturing. Through rigorous application of ISO 14040/14044-based LCA methods and correlation with process-level waste data, the research demonstrates the added value of coupling macro-scale impact assessment with micro-scale operational insights.

Key findings reveal that while conventional LCA captures broad environmental burdens such as global warming potential, toxicity, and water usage, it lacks the resolution needed to reflect the immediate material efficiency and waste generation patterns critical to process design. Conversely, green chemistry metrics offer direct, actionable feedback on material input–output dynamics but fall short of considering upstream and downstream environmental consequences. Integrating these frameworks bridges this gap, offering a dual-perspective approach that improves the identification of process hotspots, optimizes solvent recovery, and balances trade-offs between energy consumption and emissions.

The results indicate strong correlations between waste metrics and LCA categories, with higher E-factor and PMI values linked to increased environmental burdens. Notably, solvent recovery strategies reduced material waste but also raised energy demands, highlighting the importance of holistic optimization. Additionally, Atom Economy emerged as a valuable predictor of both waste minimization and impact reduction potential.

From a practical standpoint, this integrated framework provides industries with a robust toolset for advancing sustainable chemical production. It aids in benchmarking processes, guiding innovation, supporting regulatory compliance, and informing transparent sustainability reporting. Nevertheless, the study also acknowledges the ongoing challenges in standardizing waste metrics within ISO-based assessments, particularly concerning methodological consistency and data harmonization.

In conclusion, the integration of LCA with green chemistry indicators enhances the precision, relevance, and applicability of sustainability assessments in chemical engineering. It enables a more nuanced understanding of trade-offs and performance synergies, paving the way for cleaner, more efficient, and more responsible manufacturing systems. Future research should focus on refining integration techniques, expanding applicability across industrial sectors, and establishing unified reporting protocols to strengthen the practical impact of this approach.

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