

Optimizing Environmental Performance in Chemical Manufacturing: A TRACI and USEtox-Based Life Cycle Approach to Waste Minimization

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ABSTRACT: Chemical manufacturing is under increasing pressure to reduce its environmental footprint. Life Cycle Assessment (LCA), as defined by ISO 14040/14044, is an established method for evaluating such impacts. This study aims to integrate LCA with quantitative waste minimization metrics Process Mass Intensity (PMI) and E-Factor to evaluate the environmental benefits of process redesign. Two chemical process scenarios (baseline and improved) were assessed using a cradle-to-gate LCA approach. TRACI 2.1 and USEtox were employed to evaluate environmental impacts across categories such as climate change, human toxicity, and water use. PMI and E-Factor were calculated from foreground process data, and background inventory was sourced from the ecoinvent database. Allocation was based on mass, and uncertainty was assessed via Monte Carlo simulations and sensitivity analysis. The improved process demonstrated a 33% reduction in PMI and a 50% decrease in E-Factor, driven by solvent recovery and energy optimization strategies. Climate change impact dropped from 15.0 to 10.2 kg CO₂-eq, while human toxicity and water footprint also saw substantial improvements. LCA findings provided actionable insights for process redesign, revealing that targeted waste minimization enhances overall environmental performance. While energy demands initially rose, optimization and heat integration neutralized trade-offs, supporting more sustainable operations. Integrating LCA with PMI and E-Factor offers a robust, standardized framework for evaluating waste minimization in chemical processes. This approach supports environmentally sound decision-making and can guide future innovations in green chemistry and sustainable manufacturing.

Keywords: Life Cycle Assessment, Process Mass Intensity, E-Factor, Chemical Process Design, Waste Minimization, TRACI, USEtox



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INTRODUCTION

Chemical manufacturing is undergoing a critical transformation as sustainability becomes a core priority for industries worldwide. The sector faces escalating environmental challenges, including

excessive energy use, the production of hazardous waste, and considerable greenhouse gas (GHG) emissions throughout the production lifecycle. These concerns have intensified the demand for more sustainable production methods that optimize resource use and minimize environmental harm (Parvatker et al., 2019; Riazi et al., 2019). Particularly, chemical processes that result in high levels of by-products not only complicate waste management but also contribute significantly to toxicity and environmental degradation. Additionally, the shift toward bio-based feedstocks while potentially beneficial introduces new environmental trade-offs, such as land use changes and conflicts with food supply chains (Isola et al., 2017).

In response to these challenges, Life Cycle Assessment (LCA) has emerged as a robust methodological tool for assessing the environmental impacts associated with chemical manufacturing. Defined by international standards ISO 14040 and ISO 14044, LCA provides a systematic framework to evaluate emissions, resource use, and other environmental consequences across the entire lifecycle of a product from raw material extraction through production, and, in some cases, disposal (Grimaldi et al., 2021; Othman et al., 2019). By adopting a life cycle perspective, LCA enables early identification of environmental hotspots and facilitates more informed decision-making at the process design stage. This integration of environmental, technical, and economic considerations enhances not only process sustainability but also operational efficiency. Furthermore, applying LCA at pilot scales provides valuable insights into both environmental safety and economic feasibility (Zhou et al., 2017).

Despite its strengths, traditional LCA methodologies have limitations. Chief among them is the frequent omission of robust quantitative waste metrics. Without incorporating specific indicators of material efficiency and waste generation, such as Process Mass Intensity (PMI) and E-Factor, the LCA framework may fall short in providing a complete environmental profile of a chemical process (Nikolić et al., 2019). This shortfall can lead to underestimating the environmental burden of certain waste streams, particularly those associated with resource depletion and toxicity. Consequently, decision-makers may be misled about the true sustainability of a process, limiting the efficacy of environmental improvements (Barcelos et al., 2020). Scholars emphasize the necessity of integrating waste metrics into LCA to ensure more accurate, actionable, and reliable sustainability assessments (Adeoye et al., 2023; Maciel et al., 2019).

PMI and E-Factor are two of the most widely recognized metrics for evaluating material efficiency in chemical processes. PMI calculates the ratio of total mass inputs to the mass of the desired product, offering a clear measure of resource utilization (Parvatker et al., 2019; Adeoye et al., 2023). A lower PMI reflects a more efficient process with reduced material waste. The E-Factor, which quantifies the amount of waste generated per unit of product, complements PMI by providing an estimate of a process's waste intensity (Patel & Desai, 2024). Both metrics are instrumental in advancing the goals of green chemistry, enabling industries to minimize inputs and outputs, and promoting circular economy practices (Tsang et al., 2018).

To ensure methodological consistency, LCA studies are guided by ISO 14040 and ISO 14044, which standardize the procedures for conducting life cycle evaluations. These standards define four essential phases: goal and scope definition, inventory analysis, impact assessment, and

interpretation (Bisinella et al., 2021). Standardization not only enhances the transparency and reproducibility of LCA studies but also facilitates cross-sectoral comparability and regulatory compliance. Following these guidelines strengthens the credibility of LCA findings and supports their adoption in policy development and product certification (Bisinella et al., 2021).

Integrating LCA with quantitative waste minimization metrics offers multifaceted benefits for sustainable chemical manufacturing. This hybrid approach enables a more granular analysis of process sustainability by capturing both environmental impacts and operational inefficiencies. Organizations can identify and prioritize high-impact areas for improvement, leading to reduced waste, optimized resource use, and lowered operational costs (Armstrong et al., 2023). Moreover, such integration facilitates the implementation of best practices in sustainability, fostering environmental accountability and enhancing the competitive positioning of firms in environmentally sensitive markets (Abdelhalem et al., 2019). Consequently, this study aims to evaluate the environmental benefits of integrating PMI and E-Factor within an ISO-compliant LCA framework to assess two chemical process scenarios: a baseline case and an improved case incorporating waste minimization strategies.

METHOD

Life Cycle Assessment (LCA) offers a robust framework for quantifying environmental impacts across the full lifecycle of products and processes. This study employs an LCA-based comparative analysis to evaluate two process scenarios in chemical manufacturing: a baseline system and an improved system incorporating waste minimization strategies. The methodological approach is grounded in ISO 14040 and ISO 14044 standards.

Goal and Scope Definition

The primary objective of this study is to evaluate the environmental performance of two chemical production scenarios baseline and improved using cradle-to-gate boundaries. The functional unit is defined as 1 kg of product A at 99.9% purity, ensuring comparability across impact categories. According to best practices, system boundaries include all upstream and on-site processes, such as raw material extraction, transport, synthesis, energy consumption, emissions, and waste disposal (Hartmann et al., 2022).

Stakeholder engagement and an iterative scoping process were used to refine the system boundaries and objectives. When uncertainties regarding process inclusion were encountered, a provisional boundary-setting method was applied, with boundaries adjusted as more complete data became available (Li et al., 2019).

Life Cycle Inventory (LCI) Compilation

Foreground data for the LCI were collected from on-site measurements, including energy meters, process logs, and emission records. These cover inputs such as raw materials, solvents, energy,

cooling water, and emissions to air, water, and land. Background data were sourced from the ecoinvent 3.8 database.

Waste Minimization Metrics: PMI and E-Factor

The study applies two key indicators to quantify material efficiency:

- Process Mass Intensity (PMI), defined as the total mass input divided by the mass of the desired product.
- E-Factor, calculated as the ratio of waste mass to product mass, excluding water.
- These metrics allow for a more granular interpretation of waste generation in tandem with the broader LCA outputs.

Impact Assessment Methodology

Life Cycle Impact Assessment (LCIA) was conducted using two tools:

- TRACI 2.1, developed by the U.S. EPA, was applied to quantify midpoint indicators such as global warming potential, acidification, eutrophication, and photochemical smog formation.
- USEtox, a consensus model, was used to assess human toxicity and freshwater ecotoxicity, particularly relevant for processes involving solvents and hazardous intermediates.

Allocation Strategy

Processes that generated co-products used a mass-based allocation approach to distribute environmental burdens. This method aligns with ISO standards and is preferred when physical characteristics better represent functional relationships (Daystar et al., 2024). For comparison, economic allocation and system expansion were explored as sensitivity checks (Hierro et al., 2021).

Uncertainty and Sensitivity Analysis

To improve confidence in the results, the study employed multiple uncertainty assessment techniques:

- Monte Carlo Simulation: Simulated 1,000 scenarios with varying input parameters to analyze output variability.
- Sensitivity Analysis: Key parameters such as solvent recovery rate, electricity consumption, and raw material yield were varied to assess their influence on impact categories.
- Probabilistic Methods: Statistical distributions were applied to input ranges to estimate uncertainty margins in final LCIA outputs.

These integrated approaches enhance the robustness of the analysis and allow for more informed interpretation of results, supporting better decision-making in sustainable chemical process design.

RESULT AND DISCUSSION

This section presents the key findings from the Life Cycle Inventory (LCI), waste minimization metrics, and Life Cycle Impact Assessment (LCIA) for the baseline and improved chemical process scenarios. It draws on primary data collection, comparative modeling, and the use of standard tools (TRACI and USEtox).

LCI Hotspots

Life Cycle Inventory analysis reveals that energy consumption and solvent usage are the two most significant contributors to environmental impacts. In the baseline scenario, electricity usage totaled 12.0 kWh per functional unit (1 kg product), while solvent losses were recorded at 0.80 kg. These figures align with findings that energy use dominates LCA profiles in chemical manufacturing due to high energy demands for reaction and separation steps (Hanasaki et al., 2018). Similarly, solvents contribute to toxicity and air quality degradation, especially through volatile organic compounds (VOCs) (Kalvani et al., 2019).

Raw material usage and water consumption also show notable environmental footprints. The baseline system required 1.20 kg of feedstock and 5.0 m³ of cooling water, contributing to resource depletion and water stress. To visualize these hotspots, bar charts and Sankey diagrams were generated, clearly illustrating material and energy flows and highlighting areas for intervention (Schomberg et al., 2021).

Waste Minimization Metrics

Quantitative waste indicators Process Mass Intensity (PMI) and E-Factor confirm the improvements in the redesigned process. The improved scenario shows a 33% reduction in PMI (3.0 to 2.0) and a 50% drop in E-Factor (2.0 to 1.0). These values were validated through production audits, aligning with industry standards and performance thresholds (Farooq & Gheewala, 2019).

The increase in solvent recovery efficiency from 50% to 80% is particularly noteworthy. This was achieved via the integration of distillation columns and energy-efficient recovery systems, such as membrane technology and liquid-liquid extraction, supporting closed-loop solvent use (Forin et al., 2020).

LCIA Results

The LCIA results, modeled using TRACI and USEtox, indicate substantial environmental improvements in the improved scenario across all categories:

- Climate Change: Reduced from 15.0 to 10.2 kg CO₂-eq
- Acidification: Decreased from 0.35 to 0.20 kg SO₂-eq
- Eutrophication: Reduced from 0.18 to 0.10 kg N-eq

- Human Toxicity: Improved from 0.00045 to 0.00025 CTUh
- Freshwater Ecotoxicity: Lowered from 1.2 to 0.7 CTUe
- Water Footprint: Dropped from 5.0 to 3.3 m³

These results highlight the effectiveness of solvent and energy optimization. The water footprint reduction reflects better cooling efficiency and aligns with water sustainability benchmarks (Nkiaka et al., 2024). Modeling through TRACI and USEtox ensures comparability and scientific credibility (Goldstein et al., 2016).

Implications of LCIA Results for Process Design and Regulation

The LCIA findings inform both design improvements and regulatory alignment. Reductions in climate and toxicity impacts indicate that improved processes can support environmental compliance while promoting innovation (Higham et al., 2024). Moreover, the results guide designers in selecting technologies with better environmental profiles, supporting a proactive, sustainability-driven approach to chemical production.

The findings of this study underscore the effectiveness of waste minimization strategies in improving the environmental performance of chemical manufacturing. However, as demonstrated in both LCA results and supporting literature, such strategies must be assessed with a nuanced perspective, particularly due to the potential trade-offs and limitations inherent in process modifications.

One of the primary advantages of the improved process scenario lies in the integration of solvent recovery and energy optimization. These strategies successfully lowered the Process Mass Intensity (PMI) and E-Factor, alongside reductions across all impact categories modeled through TRACI and USEtox. However, it is critical to acknowledge that these improvements may introduce environmental trade-offs. For instance, implementing solvent recovery via distillation may initially increase energy requirements, particularly in the absence of integrated heat recovery systems. Such trade-offs have been identified in similar studies where waste minimization led to additional energy burdens or secondary emissions (Glogic et al., 2021; Silvestre et al., 2016). Moreover, circular practices, such as recycling, can sometimes lead to local environmental degradation if byproducts are not properly managed (Pierobon et al., 2018).

Despite these complexities, solvent recovery in this case was designed to minimize additional energy inputs by optimizing distillation sequences and integrating heat exchangers. This approach is consistent with evidence that optimized recovery can ultimately reduce net energy use when compared to sourcing virgin solvents (Khatri et al., 2021). Additionally, heat integration strategies further amplified these benefits by reclaiming energy from waste streams, lowering the overall process energy demand and fossil fuel dependency (Park & Waqar, 2022).

These findings also have important implications for process redesign. The LCA outcomes provided a clear, data-driven basis for evaluating which process improvements offered the greatest environmental benefit. For instance, reductions in climate change and human toxicity indicators guided the selection of cleaner energy sources and alternative materials. Such insights are valuable

in iterative design efforts where environmental performance must be balanced with technical and economic constraints (Saouter et al., 2017). LCA not only aids in prioritizing environmental hotspots but also fosters interdisciplinary collaboration among stakeholders in regulatory, engineering, and sustainability roles (Carvalho & Gilbertson, 2023).

Nonetheless, this study also reveals the common limitations associated with LCA methodologies. One challenge lies in the variability and uncertainty of data, particularly when background data is drawn from generalized databases rather than site-specific sources (Zhang et al., 2024). In addition, LCA tends to underrepresent socio-economic and long-term impacts such as biodiversity loss and social equity thus limiting its ability to capture the full spectrum of sustainability concerns (Greer et al., 2022). Methodological differences, such as alternative characterization models, can also lead to divergent results across similar studies. Addressing these issues will require continued advancements in LCA tools, databases, and interdisciplinary frameworks, possibly through integration with other assessment methodologies (Pourzahedi et al., 2017).

In summary, while waste minimization strategies such as solvent recovery and energy optimization offer substantial environmental gains, their implementation must be guided by holistic LCA evaluations. Balancing direct environmental benefits against potential trade-offs enables more informed and responsible decision-making in sustainable chemical process design.

CONCLUSION

This study has demonstrated that integrating waste minimization strategies into chemical process design can significantly reduce environmental burdens, particularly when guided by ISO-compliant Life Cycle Assessment (LCA) and quantitative efficiency metrics such as Process Mass Intensity (PMI) and E-Factor. Through a comparative analysis of a baseline process and an improved scenario, key environmental impact categories including climate change, human toxicity, and water usage were measurably reduced. Specifically, the improved process scenario resulted in a 33% reduction in PMI, a 50% reduction in E-Factor, and marked declines in LCIA categories modeled using TRACI and USEtox.

The integration of solvent recovery and heat integration proved to be effective in reducing emissions and resource consumption, despite initial concerns about energy trade-offs. The study found that with process optimization, these strategies contributed to net environmental benefits, enhancing both material and energy efficiency. Moreover, the use of standardized impact assessment tools allowed for consistent comparison across scenarios, supporting informed decision-making.

Beyond these technical outcomes, the study contributes a structured methodological framework for combining waste metrics with LCA, offering a replicable model for process designers, sustainability practitioners, and regulatory bodies. It reinforces the role of LCA not just as a reporting tool, but as a proactive instrument for guiding sustainable innovation in the chemical industry.

Future research should aim to incorporate broader system boundaries such as cradle-to-grave perspectives and examine socio-economic and biodiversity impacts currently underrepresented in LCA. Furthermore, applying this framework to different chemical sectors will help validate its generalizability and support continuous improvement in sustainable process development.

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