Master Thesis Concept: Comparing and Connecting Green Chemistry Metrics with LCA Indicators

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Research Objectives

- Conduct a comprehensive literature review on green chemistry metrics and life cycle assessment (LCA) indicators, highlighting their definitions, scopes, and applications.
- Investigate methodologies for calculating key green chemistry and LCA metrics, including data requirements and computational approaches.
- Identify and evaluate relevant datasets for metric calculation, with a focus on established databases such as Ecoinvent.
- Apply data analysis and data science tools to analyze, compare, and correlate green chemistry metrics with LCA indicators.
- Provide an extended overview of these metrics and propose a framework or guidelines for their integrated use in sustainability assessment.
- Demonstrate the practical utility of the integrated approach through selected use cases in chemical processes or product development.

Research Questions

1. **What are the main green chemistry metrics and LCA indicators used to assess the sustainability of chemical products and processes?**
2. **How are these metrics calculated, and what are the methodological differences and complementarities between them?**
3. **Which datasets (e.g., Ecoinvent) and data sources are suitable and available for calculating these metrics reliably?**

4. **What are the correlations and discrepancies between green chemistry metrics and LCA indicators based on data analysis?**
5. **How can data science techniques enhance the understanding and integration of these metrics?**
6. **What practical examples or case studies illustrate the benefits and challenges of combining green chemistry metrics with LCA indicators?**

Literature Review Focus

- Overview of **green chemistry metrics**: E-factor, atom economy, process mass intensity, energy intensity, DOZN 2.0 scores, hybridized sustainability metrics including resource circularity and hazardous chemical use[1][2][3][4][5][6].
- Overview of **LCA indicators**: life cycle impact assessment (LCIA) methods such as ILCD Midpoint+, Cumulative Energy Demand (CED), and other environmental impact categories (climate change, toxicity, resource use)[1][7][3][8].
- Comparative studies highlighting strengths and limitations of green chemistry metrics vs. LCA, and the need for integrated approaches[1][2][7][6].
- Data challenges and opportunities, including the use of **Ecoinvent** and other LCA databases for life cycle inventory data[8].
- Recent advances in hybridized metrics combining green chemistry principles with LCA for circular economy and bio-based products[4][9].

Methodology

- **Data Collection**: Extract data from literature, public LCA databases (e.g., Ecoinvent), and case studies for chemical processes.
- **Metric Calculation**: Implement calculations of green chemistry metrics and LCA indicators using software tools (e.g., SimaPro, openLCA) and custom scripts (Python, R).
- **Data Analysis**: Use statistical analysis, correlation analysis, and machine learning techniques to explore relationships and discrepancies between metrics.
- **Visualization**: Develop visual tools (e.g., heatmaps, scatter plots) to illustrate metric comparisons and patterns.

- **Case Studies**: Select representative chemical syntheses or products (e.g., bio-based vs. petrochemical routes, organic molecules) to apply and validate the integrated metric framework[8].

Tools and Techniques

- Life Cycle Assessment software: **SimaPro**, **Activity Browser, Makersite**
- Programming languages and libraries: **Python** (pandas, numpy, scikit-learn, matplotlib), **R**
- Data analysis and visualization techniques: correlation matrices, principal component analysis (PCA), clustering, etc.
- Access to databases: **Ecoinvent**, literature datasets

Potential Use Cases

- Comparing alternative synthetic routes for a chemical product using both green chemistry metrics and LCA indicators to identify the most sustainable option[8].
- Evaluating bio-based versus fossil-based product supply chains with hybridized metrics that incorporate resource circularity and hazardous chemical use[4][9].
- Assessing the environmental impact and resource efficiency of emerging green technologies in chemical manufacturing.
- Developing decision-support frameworks for researchers and industry to apply integrated sustainability metrics early in process design.

Expected Contributions

- A detailed synthesis of green chemistry and LCA metrics, clarifying their roles in sustainability assessment.
- A practical methodology for calculating and comparing these metrics using real-world data.
- Insights into the correlation and complementarity of green chemistry metrics and LCA indicators.
- Demonstration of data science techniques enhancing metric integration and interpretation.

- Recommendations for researchers and practitioners on applying combined metrics for greener chemical innovation.

This concept leverages recent scholarly insights emphasizing the need to integrate mass- and energy-based green chemistry metrics with comprehensive LCA indicators to achieve more robust sustainability assessments, supported by data science methods and real datasets like Ecoinvent[1][2][3][4][8][6].

1. https://onlinelibrary.wiley.com/doi/pdf/10.1002/cite.202300229
2. https://onlinelibrary.wiley.com/doi/10.1002/cite.202300229
3. https://pubs.rsc.org/en/content/articlepdf/2021/gc/d1gc02623b
4. https://pdfs.semanticscholar.org/8094/416f3353e7af1e191c765d2c407dee53c0b4.pdf
5. https://pmc.ncbi.nlm.nih.gov/articles/PMC8667789/
6. https://pubs.rsc.org/en/content/articlelanding/2024/gc/d4gc00394b
7. https://scite.ai/reports/assessment-of-chemical-products-and-wm0aYa9l
8. https://www.frontiersin.org/journals/chemistry/articles/10.3389/fchem.2020.00214/full
9. https://eprints.whiterose.ac.uk/id/eprint/155654/1/c9gc02992c.pdf