Exercise 3: Performing a simplified LCA study for chemicals

Assume that your group is advising a product manager at “GreenPoly Solutions” in the search for a new raw material in the making of a product that your company is manufacturing. All five alternatives at this point so far meet the performance and cost criteria, but you also want to lower the carbon footprint of your product portfolio. Perform a pragmatic, streamlined Life Cycle Assessment (LCA) of at least three of the five alternatives and try to come to a recommendation for your management.

Put your results into a concise and transparently documented short report (up to 10 text pages, excluding title pages, figures, references and appendices – less is better). Collect strongly simplified energy and mass balances for your work in a standardized format. Use any means you can to come up with a solid recommendation for your management (including e.g. generative AI). Make sure that the results are technically correct and sound. Guiding questions and hints for the report are attached as appendix A. Some potentially useful background data and papers are provided in appendix B. The grading scheme is provided in appendix C.

For the final submission, please make sure that all members of the team are listed on the title page (with their matriculation numbers and email addresses). The deadline for submission is at the end of the semester with the other exercises. Please submit your final report, your calculation files and your collected data.

Appendix A - Hints and guiding questions:

1. Start by getting to know the applications of your chemicals and try to figure out which candidates you would like to work on. Starting the data work with a more straightforward chemical can inform the selection of the others.
2. Think about the functional unit. How much of each product is equivalent to the others?
3. What are the system boundaries of your analysis? What is included and what not (raw materials extraction, manufacturing, distribution, use phase, waste treatment, etc.)? Consider neglecting life cycle stages in which you expect limited differences between chemical products.
4. What is the regional and temporal scope of your analysis? Consider that base chemical manufacturing is hardly taking place in Switzerland.
5. Try developing a realistic manufacturing chain from the final products to known precursor substances in the IDEMAT LCI database that correspond to your regional and temporal scope.
6. For each step in your manufacturing chain, try to collect mass and energy balances in a standardized format. Apply similar assumptions where possible. Focus on one manufacturing route per chemical that you consider most representative and make use of overlaps in the products where possible.
7. Try to estimate mass balances based on known data, estimate it from similar reactions if there is no known data, or else employ simplified realistic assumptions. Whenever something would consume considerable amount of time in preparation, think about more pragmatic solutions, that could still lead to meaningful results.
8. For energy balances, try to estimate them based on simplified calculation procedures, but also consider reported balances or similar reactions if they are reported, possibly by adjusting them to your use case.
9. Try to figure out if the chemicals are likely to be produced in efficient continuous processes with energy recovery or at smaller scale without energy recovery. Similarly, think about whether any outputs are likely co-product with significant commercial value or rather a waste that is to be treated (also considering the scale of manufacturing).
10. In cases of by-products, apply a consistent allocation approach to attribute impacts for multi-output processes, and argue why it is suitable for your use case.
11. Reflect on the fate of wastes that are generated for example during production and apply simplified waste treatment approaches per type (waste water treatment, incineration, landfilling, etc.). Do not forget to add relevant greenhouse gas emissions.
12. Do any of the chemical reactions involve the formation of greenhouse gases such as CO2, CH4 or N2O? If so, try to figure out if they are usually abated or not in your regional or temporal scope (e.g. N2O catalyst, combustion) and add them to your inventories.
13. Select suitable dataset for the main utility supplies (electricity, steam, fuels, cooling, gases, etc.) and add them to your inventories.
14. Calculate cumulative inputs and outputs for each of your products for the entire system within the system boundaries.
15. Add estimates from climate change impacts (using the IPCC GWP 100a method) for the inputs and outputs.
16. Interpret the results. What is influential in the LCA of each product and what is not? How do the products compare against each other? Are the results plausible in comparison to similar products?
17. What creates major uncertainty in your results? What data or methods would be needed to reduce the uncertainty? Can all types of uncertainty be reduced or not?
18. What would you recommend to the product manager at “GreenPoly Solutions”? What would you communicate as the confidence level of your results?

Appendix B – Data sources and methods

IDEMAT database with baseline GWP 100a data for energy, basic chemicals, waste treatment, etc.:
https://www.ecocostsvalue.com/data-tools-books/

IDEMAT tool for simplified LCA calculations (optional use):
https://www.ecocostsvalue.com/data-tools-books/tool-in-excel/

WIPO patent search (e.g. if you know the inventor or manufacturer of a chemical):
https://patentscope.wipo.int/search/en/search.jsf

Reaxys (properties/features of reactions like yields, temperatures):
https://www.reaxys.com/#/search/quick/query

ULLMANN'S Encyclopedia of Industrial Chemistry (for manufacturing background information):
https://onlinelibrary.wiley.com/doi/book/10.1002/14356007

Kirk-Othmer Encyclopedia of Chemical Technology (for manufacturing background information):
https://onlinelibrary.wiley.com/doi/book/10.1002/0471238961

Paper on a basic approach for estimating life cycle inventories for chemicals:
https://link.springer.com/article/10.1007/BF02978615

Pharmaceuticals LCI examples (fine chemicals, batch processes)
https://pubs.acs.org/doi/full/10.1021/acssuschemeng.8b05473

Gate-to-gate process energy demands (bulk chemicals, continuous processes):
https://pubs.acs.org/doi/10.1021/acssuschemeng.0c00439

Energy demand averages for processes (as fallback for lack of more meaningful data):
https://scijournals.onlinelibrary.wiley.com/doi/full/10.1002/jctb.821

IPCC GWP 100a characterization factor values:
https://ghgprotocol.org/sites/default/files/2024-08/Global-Warming-Potential-Values%20%28August%202024%29.pdf

Default GHG emission factors for the combustion of various fuels:
https://www.ipcc-nggip.iges.or.jp/public/2006gl/pdf/2_Volume2/V2_2_Ch2_Stationary_Combustion.pdf#page=18

Default net calorific values for various fuels:
https://www.ipcc-nggip.iges.or.jp/public/2006gl/pdf/2_Volume2/V2_1_Ch1_Introduction.pdf#page=18

ECHA data on production/import tonnage in the EU for an idea of the scale of manufacturing:
https://echa.europa.eu/information-on-chemicals/registered-substances

OECD list of high production volume chemicals (>1000 tonnes per year):
https://one.oecd.org/document/ENV/JM/MONO(2007)28/en/pdf

Appendix C – Grading scheme (up to 60 points in total starting from 10, low quality = add 0 pts, medium = 1 pt, high = 2 pts per item, up to 10 bonus points, converted to grade by dividing by 10):

1. Plausible functional unit
2. System boundary clear and sensible
3. Concise and understandable writing style
4. Documentation of general approach
5. Documentation of calculations
6. Documentation of data sources
7. Consistent approach across alternatives
8. Clear and understandable graphics
9. Easy to read and understand
10. Logically structured text
11. Standardized data collection
12. Full data and calculations submitted
13. Realistic results obtained
14. Plausibility check performed
15. Uncertainties, gaps and limitations discussed
16. Meaningful life cycle stages covered
17. Regional and temporal scope defined
18. Mass balances before allocation are closed
19. Suitable datasets from LCI databases selected
20. Recommendations/conclusions make sense
21. Correct technical language used
22. Waste treatment covered
23. Meaningful simplifications and shortcuts
24. Drivers of impacts analyzed
25. Allocation in case of co-products explained

Bonus points

Note: There may still be minor adjustments to the grading scheme if we see the need for that.