Automating Life Cycle Assessment from Chemical Process Simulations

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Abstract

Advancing sustainability requires knowledge on the environmental impacts of chemicals. For this purpose, life cycle assessment is the preferred method, but usually carried out by manually extracting data from process simulation software and transferring data to life cycle assessment software. This process is very labor-intensive and error-prone.

Here, we bridge the gap between process simulation and life cycle assessment by automated data extraction from process simulators to life cycle assessment software. Our tool currently links the process simulators Aspen Plus, Aspen HYSYS, and AVEVA Process Simulation to the open-source tools Brightway/Activity Browser for life cycle assessment. The tool is exemplified using openly available case studies and simulation files for bio-based and CO2-based processes. Simulation studies can be combined to, e.g., integrated CO2 capture and utilization chains within life cycle assessment software.

Our tool directly integrates process simulations results into life cycle inventory databases with easy workflows and could thereby enable the generation of more life cycle assessments of chemical processes.

**Keywords**: chemical process simulation, life cycle assessment, automated data extraction, life cycle inventory

* 1. Introduction

Life cycle assessment (LCA) of chemical processes is a crucial part of process development [(Hungerbühler et al., 2021)](#_CTVL001bb692cf2273f48c7b3f7837dccc2f937). Often, LCA is performed subsequent to process development and simulation (Köck et al., 2023). Today, the LCA computation relies on manual data handling for transferring simulation results to life cycle assessment software and requires deep process knowledge [(Köck et al., 2023)](#_CTVL001e132954e29934c8eb0af9a337800c421). This approach is labor-intense and error-prone [(Azzaro-Pantel et al., 2022)](#_CTVL0019ce8a538651f43a788f3777fac5edbd7) and might neglect flows that seem irrelevant but substantially contribute to environmental impacts [(Rosental et al., 2020)](#_CTVL001a7a3f7f7cdbc4d8bb3ea3cd2d9e757cf). However, the workflow of LCA for chemical processes offers the potential for standardization, as many chemical processes follow a logic of converting feedstocks to products, byproducts, and waste with the help of utilities and solvents [(Hungerbühler et al., 2021)](#_CTVL001bb692cf2273f48c7b3f7837dccc2f937). Therefore, streamlining the workflow can significantly ease and accelerate the LCAs of chemical processes.

In this work, we establish a bridge between process simulation and LCA by introducing an automated data extraction tool that connects the process simulation software Aspen Plus [(Aspen Technology Inc., 2019a)](#_CTVL001f9a22aa8de6940d68156045d9a83665d), Aspen HYSYS [(Aspen Technology Inc., 2019b)](#_CTVL001a9599dadaa254afab225834c6f4917d5), and AVEVA Process Simulation [(AVEVA Group plc, 2023)](#_CTVL001bf169aa33b314572919e4b6243c3f7e6) with the LCA software Brightway [(Mutel, 2017)](#_CTVL00143d4d791912843c2ad3e80903509aac5). Our tool simplifies the integration of standard software and methodologies in process systems engineering with the tools essential for LCA. Automating data processing accelerates the LCA process, facilitating the integration into larger systems and limiting the possibility of data transfer errors.

* 1. Methods

Our tool streamlines the connection of process simulation to LCA. For this purpose, we connect common process simulators with the open-source Python-based software package Brightway [(Mutel, 2017)](#_CTVL00143d4d791912843c2ad3e80903509aac5), a well-established and widely adopted tool within the academic LCA community. Furthermore, integration into Brighway allows the use of the open-source LCA tool Activity Browser, which offers an intuitive graphical interface for conducting additional calculations and managing databases and results [(Steubing et al., 2020)](#_CTVL001d84b337e425e4d02b25443c68dc08d54). By using Python as a shared programming language across both process simulation and LCA domains, we ensure a unified and cohesive approach to our implementation. A graphical user interface guides the user through the workflow, from flowsheet extraction to life cycle inventories (LCIs) and life cycle impact assessment (LCIA).

In its current implementation, our tool supports the process simulation software Aspen Plus [(Aspen Technology Inc., 2019a)](#_CTVL001f9a22aa8de6940d68156045d9a83665d), Aspen HYSYS [(Aspen Technology Inc., 2019b)](#_CTVL001a9599dadaa254afab225834c6f4917d5), and AVEVA Process Simulation [(AVEVA Group plc, 2023)](#_CTVL001bf169aa33b314572919e4b6243c3f7e6), which are common software in chemical process simulation both in academia and industry [(de Beer and Depew, 2021)](#_CTVL0017a9c70f83fff4cd5aab5428f254a740b). The only input to the extraction tool is a simulation file of a chemical process, which is evaluated and from which all mass and energy streams are extracted.

After extracting process simulation results, the next step involves linking the process streams with the corresponding activities in life cycle assessment databases to calculate environmental impacts. Typically, life cycle inventory databases such as ecoinvent [(Wernet et al., 2016)](#_CTVL001d71f9b7c427b4885b46cbb7c34911bbb) or GaBi [(Sphera Solutions Inc., 2023)](#_CTVL00180ebd2e0ad1a4005afdd3fe928a094cb) are used. The process streams are either linked to direct emissions to the environment or linked to activities further down the supply chain, which causes underlying environmental impact. The stream-linking step requires manual user input and is hard to automate since specifications are needed for the exact locations, energy mixes, or modeling assumptions, e.g., options for waste treatment. However, the user is assisted by a graphical interface providing process streams and life cycle inventory activities next to each other in one combined interface for easy linking. Furthermore, the user is provided with stream information and can further modify the process data. Finally, all process streams are linked to inventory activities as the final step of the life cycle inventory analysis (LCI).

Starting from the LCI, the life cycle impact assessment (LCIA) is calculated automatically to determine the potential environmental impacts of the investigated process. Furthermore, the contribution of the streams to the overall impacts in various impact categories is evaluated. The contribution analysis allows for identifying hotspots that might require further process development. Finally, LCI and LCIA results can be exported and used further in other simulations. As the results are stored within Brightway, newly developed processes can be integrated and evaluated in larger supply chains.

* 1. Case Study

The robustness of our automated data extraction and LCA tool is tested by assessing literature case studies. These studies encompass a spectrum of processes, including bio-based conversion, CO2 capture, and CO2 utilization, for which simulation files are readily available online together with the corresponding publication or provided as example files for the process simulation software. Moreover, these studies provide access to life cycle inventories, LCA results, and/or techno-economic analysis (TEA) findings, offering a data source for validation. The simulation files were taken from the literature with no further modification. In particular, the simulations used different unit sets or stream definitions.

We demonstrate the possibilities arising from the full integration capabilities of our tool by combining multiple simulation files from three different software tools into one larger LCA study. The combination shows the potential for data handling without manual data transfer or manipulation. We combine the amine-based CO2 flue gas capture by Adams et al. [(Adams et al., 2014](#_CTVL001feb78ea400a04d6b98eb75c4dd7c0e37)[, Adams, 2017)](#_CTVL001b4a850d94a6d483abf0e707a6c68bd1d) implemented in Aspen Plus with water electrolysis provided as AVEVA Process Simulation example [(AVEVA Group plc, 2023)](#_CTVL001bf169aa33b314572919e4b6243c3f7e6) as feedstocks for the CO2 hydrogenation to methanol implemented in Aspen HYSYS [(Vázquez and Guillén-Gosálbez, 2021)](#_CTVL001ecca54c6f6bf422686b30f1e7aa8af8b) (see Figure 1).

Figure 1: Simulation files automatically combined to generate the life cycle inventory for the CO2 hydrogenation to methanol including CO2 capture and water electrolysis.



Our demonstration is executed using the ecoinvent 3.9.1 database (cutoff system model) [(Wernet et al., 2016)](#_CTVL001d71f9b7c427b4885b46cbb7c34911bbb) and the environmental footprint methodology 3.1 [(Andreasi Bassi et al., 2023)](#_CTVL0010349245f2d9a474d85f335dff4cf3a69) as life cycle inventory database and life cycle impact assessment method, respectively. For the simplicity of demonstration, only the available ecoinvent processes for the US are used, and no further modeling of feedstock or utility systems is performed.

* 1. Results

The case study demonstrates the automated integration of multiple case studies into one larger supply chain for which LCA results are automatically computed. The tool determines the total climate change impacts of methanol production to   
22.7 kgCO2eq/kgMeOH. The relative contributions to climate change impacts for methanol production are shown in Figure 2.

The tool allows for the identification of hotspots further down the supply chain and across the integrated flowsheets. Here, the major hotspot is the electricity demand for hydrogen production. In this case study, electricity is assumed to be taken from the US-average electricity grid. This assumption leads to the high climate change impacts of methanol.

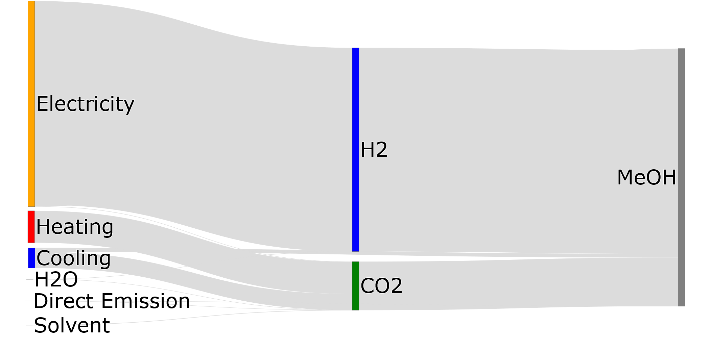


Figure 2: Relative contribution to climate change impacts for the CCU pathway to methanol by integrating the flowsheets in Figure 1.

Integrating our tool with standard software facilitates the transfer of results and the incorporation of individual processes into supply chains within the Brightway framework. Therefore, the impact of flowsheet changes on the LCA results of whole value chains can be evaluated automatically.

* 1. Conclusions

This work presents an automated data extraction tool for connecting process simulation software and life cycle assessment software. The tool showcases its capabilities by automatically integrating case studies from the literature into a comprehensive supply chain. Data handling and the calculation of environmental impacts are automated, and hotspots in the process can be identified easily.

Our methodological approach allows for the direct integration of LCI results into databases, promoting user-friendly workflows. This approach holds the potential to mitigate data gaps within life cycle inventories of chemical supply chains, facilitating more comprehensive LCAs of chemical processes. Furthermore, our tool aids the integrated development and environmental assessment of chemical processes.

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