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Life Cycle and Sustainability Analyses for Designing Chemical Circular Economy

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ABSTRACT

Sustainability and circular economy enclose initiatives to achieve economic systems and industrial value chains by improving resource use, productivity, reuse, recycling, pollution prevention, and minimizing disposed material. However, shifting from the traditional linear economic production system to a circular economy is challenging. One of the most significant hurdles is the absence of sustainable end-of-life (EoL)/manufacturing loops for recycling and recovering material while minimizing negative impacts on human health and the environment. Overcoming these challenges is critical in returning materials to upstream life cycle stage facilities such as manufacturing. Chemical flow analysis (CFA), sustainability evaluation, and process systems engineering (PSE) can supply chemical products and processes performances from environmental, economic, material efficiency, energy footprint, and technology perspectives. These holistic evaluation techniques can improve productivity, source material reduction, reuse, recycling, and prevent and minimize releases and disposal rates. Therefore, this contribution offers a computational framework that covers CFA, sustainability assessment, and risk evaluation for quantifying the benefits and challenges of chemical circular economy routes versus conventional linear systems. Finally, this contribution shows promising techniques and challenges for employing CFA, sustainability evaluation, and PSE as multicriteria decision-making tools for designing a closed-loop chemical management infrastructure and transforming the US chemical industry sector from linear to circular.

Keywords: Supply Chain, Life Cycle Analysis, Modelling, Machine Learning, Wastewater

INTRODUCTION

Tracking Chemicals and Releases at Industrial End-of-Life Activities

The Frank R. Lautenberg Chemical Safety for the 21st Century Act amended Toxic Substances Control Act (TSCA) instructs the US Environmental Protection Agency (USEPA) to conduct risk evaluations of existing high-priority chemicals to find whether a chemical substance in the US market may pose an unreasonable risk of harming the environment or human health across its life cycle stages (manufacturing, use, end-of-life (EoL)) [1]. Therefore, chemical risk evaluation supports alternative assessments of selecting chemicals and materials with safer profiles and ensures sustainable circular economy paths (recycling, reusing, and recovering processes). However, the list of registered chemicals used in US commerce continuously grows. Also, data gathering, reconciliation, and management for performing life cycle risk evaluation are time-consuming and challenging. Notably, evaluating the chemical risk and safety at its EoL stage is more difficult due to high uncertainty, less data availability, variability, material blends, and the absence of directing requirements for proper reporting and traceability.

Several efforts aim to create a data engineering framework for building an EoL database and tracking chemicals at their EoL stage. This framework performs a data engineering procedure to gather, clean, wrangle, and integrate information from publicly available USEPA databases such as the Toxics Release Inventory (TRI), the Facility Registry Service (FRS), and the Substance Registry Services (SRS). Furthermore, the framework supports data cleaning, filtering, filling data gaps, and transformation into machine-readable queries to address and enhance chemical risk evaluation of chemicals of concern.

As described in **Figure 1**, the first module of the EoL framework addresses EoL flows generated by industrial facilities (manufacturing and industrial use life-cycle stages) and transferred for further EoL management at recycling, energy recovery, treatment, and disposal facilities (RETDFs). Also, a case study of methylene chloride (dichloromethane) showed the practicality of the developed framework for tracking and analyzing EoL chemical flows from the generator industry sector of a chemical (e.g., inorganic chemical manufacturing), conditions of use (e.g., reactant, formulation component, products), the EoL facility industry sector (e.g., cement manufacturing), EoL activity (e.g., recycling, incineration, landfill), and the environmental compartment (e.g., net recycling, onsite soil releases, etc.), and estimating potential releases at EoL activities [1].

Moreover, Hernandez-Betancur et al. (2021b) enhanced the data engineering framework by using EoL pollution abatement units (PAU)-level information, chemical process design, and equipment performance data for calculating emission factors and distributing releases [2]. On-site EoL activities consist of PAUs like distillation, aerobic treatment, neutralization, incinerator, etc. The enhanced framework also offers structure design alternatives, efficiencies, chemical releases, exposure media, operating expenses, and capital expenditures for the PAU operations.

Although the developed data engineering framework estimates EoL industrial releases and distribution, it must supply potential circular economy paths and destination of recycled/recovered chemical flows transferred to upstream chemical life cycle stage facilities (e.g., manufacturing).

METHODOLOGY

Data Analytics Techniques Supporting Safer Circular Economy Paths

The presence of chemicals causing significant adverse human health and environmental effects during EoL stages is a challenge for implementing sustainable materials management efforts towards a circular life-cycle path of chemicals. Therefore, conducting chemical risk evaluation and exposure assessment of potential EoL scenarios can aid the understanding of the chemical EoL management chain for its safer use in a circular life-cycle

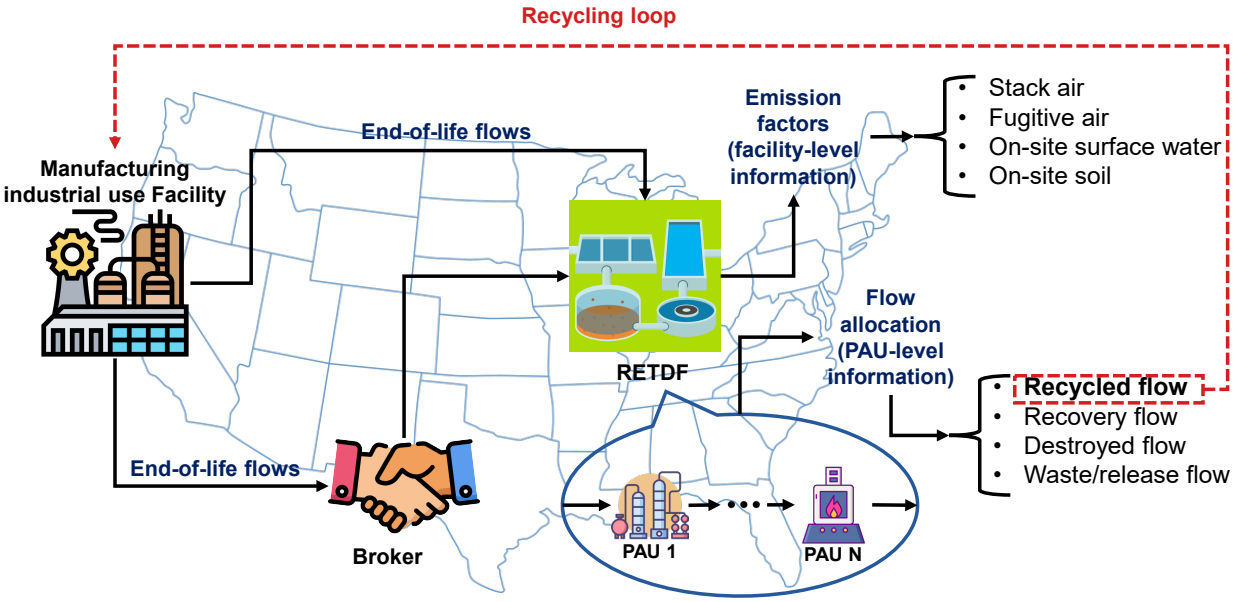


Figure 1. A data engineering framework for tracking end-of-life (EoL) chemical transfers to recycling, energy recovery, treatment & disposal facilities (RETDFs) for EoL management, on-site EoL industrial operations (pollution abatement units, PAU), and recycling loops (adapted from Hernandez-Betancur et al. [3])

environment.

Thus, we enhanced the data engineering framework by implementing probabilistic graphical models like Markov random field to mimic the relationship between the chemical EoL management components like the EoL flow generators, RETDFs, and manufacturing facilities [3]. The updated framework finds potential safer circular economy scenarios for recycled chemicals. These circular economy scenarios consider whether the recycled chemical might end up in industrial, commercial, consumer uses, and processing operations. Additionally, the framework can find if the recycling activities target the chemical under analysis instead of managing other chemical substances, such as the EoL multicomponent material flow transfers. The novel approach also considers regulatory constraints on closing the recycling loop operations and supplies an estimation of environmental releases related to occupational exposure.

RESULTS AND DISCUSSION

Completing life cycle and sustainability analyses requires adapting different strategies based on the varying levels of information available. In this computational framework, data-driven model systems may be used to accurately track and predict material pathways throughout the life cycle when process, chemical, and material exchange information are available in larger quantities. Conversely, chemical flow analysis (CFA) may be used to qualitatively map the allocation of chemicals and quantify the relative mass flow distribution across EoL pathways and technologies. The output of these material tracking methods can establish a basis for sustainability analysis because the process efficiency and material releases can be calculated. With sufficient process-level information, PSE models can enhance the granularity of the chemical release approximation, such as releases from individual process units. Subsequently, the operation details can be acquired and used to identify the potential occupational exposure scenarios and areas of improvement throughout a chemical life cycle analysis to achieve a circular economy.

Data-Driven Model Systems to Estimate Releases from Novel Chemical End-of-Life Scenarios

Hernandez-Betancur et al. (2023a) enhanced the EoL database by integrating cross-year and country data and considering the change of the regulatory foundations across different geographical locations and reporting years [4]. Thus, the data engineering framework is scalable and adaptable to develop machine learning (ML) models for predicting potential EoL activities, chemical flow allocation, environmental releases, and exposure routes for chemicals outside the comprehensive EoL database.

Hernandez-Betancur et al. (2023b) utilized the EoL database created by Hernandez-Betancur et al. (2023a) to investigate tree-based ML algorithms to construct an EoL release modeling approach influenced by Quantitative Structure-Activity Relationship (QSAR) models often used in cheminformatics and toxicology research [5]. In addition, the developed ML models use chemical descriptors, EoL chemical transfer quantities, industry sectors, environmental policies, industry-sector value-added, chemical structure, and chemical prices to predict potential EoL activities and the chemical transfer distribution among the EoL activities. Therefore, these ML models aid early stage chemical process/product designers in deciding if chemical substances at their potential EoL stage meet environmental regulations or need redesign before entering the market.

Although these data-driven developments based on top-down facility information aid the tracking and estimation of EoL chemical releases and finding potential occupational exposure routes, decision-makers would need to incorporate PSE methods and tools to design and evaluate chemical processes and implement enhancements to minimize or end negative environmental and economic impacts at process equipment level toward a more holistic sustainable performance (bottom-up approach).

Process Systems Engineering to Estimate Releases and Evaluate Sustainability from Chemical End-of-Life Scenarios

Chemical process synthesis, design, modeling, and simulation developments aid stakeholders in performing CFA, occupational exposure, energy footprint, release estimation, and life cycle inventory generation during EoL chemical stages. For example, Chea et al. (2023) performed a qualitative and quantitative tracking of plastic chemical additives to estimate their potential environmental releases, life cycle inventories, occupational exposure, greenhouse gas emissions, energy footprint, and environmental impacts within the plastic EoL stage and activities [6]. Also, this work shows a sensitivity analysis of future chemical additive release scenarios involving chemical recycling, increasing recycling rates, and chemical additive extraction. To complement these PSE applications, Agbleze et al. (2023) showed recent efforts to estimate chemical releases and evaluate sustainability indicators at the chemical manufacturing stage of existing chemicals, new manufacturing processes, and dynamic operating conditions [7]. Also, this contribution describes how to apply the Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator (GREENSCOPE) sustainability assessment tool to evaluate the sustainability

of chemicals synthesized from a laboratory-scale reaction or manufactured in a plant-scale reaction [8], [9]. GREENSCOPE quantifies and assesses the sustainability of a given process or supply from a multi-stakeholder perspective, including material efficiency, environmental impacts, energy requirements, and cost through mathematical indicators.

Finally, after describing recent PSE applications on EoL material flow analysis for supporting chemical risk assessment, sustainability evaluation, and safer circular economy paths, the subsequent sections describe crucial PSE applications for managing the EoL stage of novel product manufacturing techniques like additive manufacturing (AM) and quantifying and tracking chemical releases in unconventional EoL paths like publicly owned treatment works (POTWs). These efforts aid decision-makers in finding new potential chemical exposure routes and updating regulatory requirements due to ineffective EoL chemical management methods.

Shifting Additive Manufacturing End-of-Life Management Toward a Circular Economy

AM techniques have been widely used to create customized products and parts from a multitude of raw material types with high efficiency [10], [11]. However, most attention toward AM challenges is centered on the manufacturing stage of the material life cycle, emphasizing releases and occupational hazards [12]–[14]. Achieving sustainability and the state of a circular economy within a given supply chain requires that the fate of all materials used is accounted for throughout the life cycle.

Presently, AM practices can result in potential releases to the environmental compartments, namely land, water, and air, and creating new exposure pathways in the EoL stage if unmitigated. The variety of materials used during the manufacturing stage creates high uncertainties on the fate of the materials. Solid materials for EoL management ultimately combine with conventional municipal solid waste (MSW) management infrastructure at the forefront of AM material management, while liquid EoL materials are treated as hazardous waste. Releases from the manufacturing stage can go unreported because improper EoL chemical management methods or cleaning practices were used or the total releases at individual operation sites are lower than the reporting thresholds.

The GREENSCOPE tool was used to find specific challenges and process modification opportunities within the EoL stage of the AM life cycle. The calculated indicators were compared against best- and worst-case scenario values to compute a sustainability percent score ranging from 0 to 100%, in which a 100% score signifies the best sustainability scenario. **Figure 2** illustrates the sustainability analysis, summarizing concerns on the low recycling rate of AM EoL materials and the inherently low

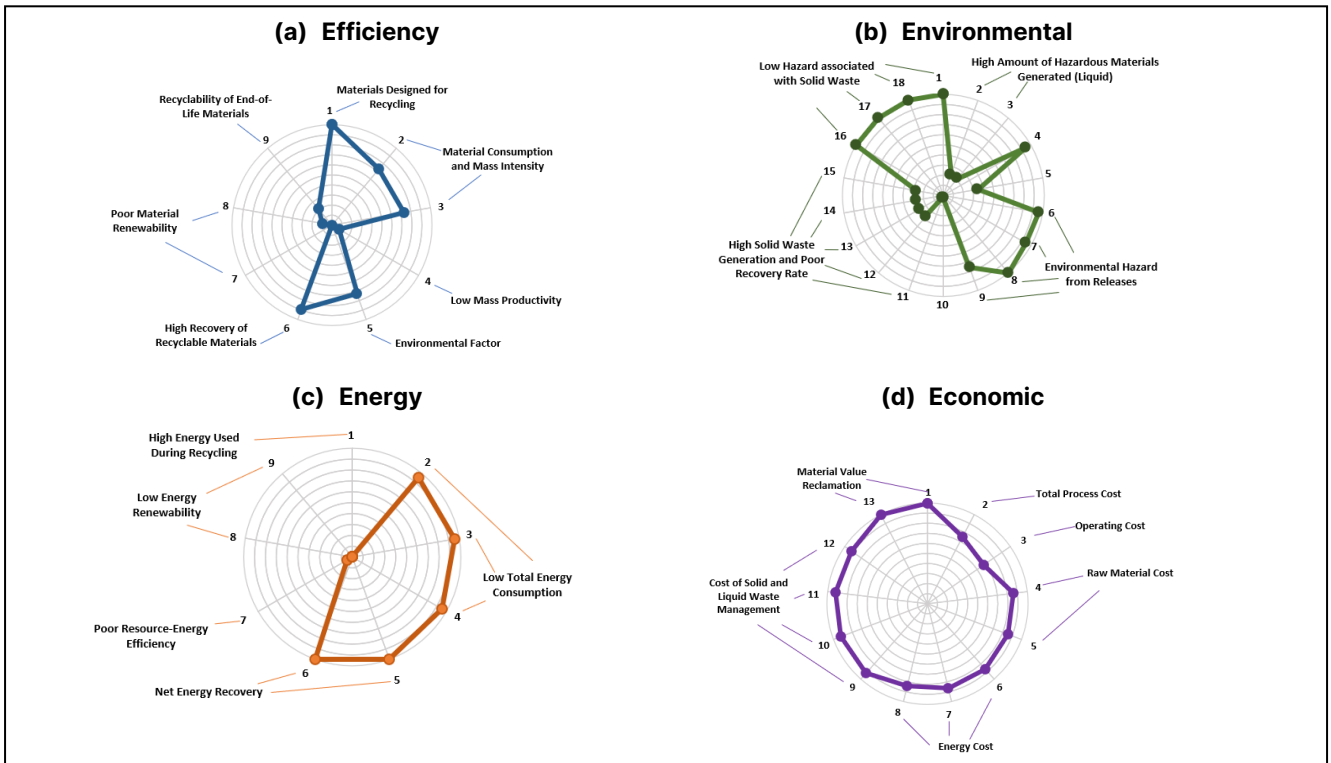


Figure 2. GREENSCOPE analysis of additive manufacturing end-of-life material management. Numerical values at the plot radii represent calculated metrics related to their respective categories. Points at the radius of each plot signify a maximum sustainability score of 100%.

renewability. The overall AM life cycle also generates a high amount of hazardous EoL materials and their releases to the environment. The total energy consumption is relatively low, but the renewability of the energy source requires improvement. Alternatively, the various cost aspects of AM EoL management processes are close to optimality. However, variation can be expected because the management infrastructure varies between regions, in addition to the variety in material types expected from releases and the manufacturing stage.

Tracking and Estimating Industrial Wastewater Transfers to Publicly Owned Treatment Works

The influx of industrial wastewater with conventional and emerging chemical contaminants to POTWs poses potential exposure risks, leading to environmental impacts and human health risks caused by polluted water discharges, land depositions, and air releases. Quantifying and tracking industrial chemical releases to POTWs are necessary to find unaddressed potential exposure routes. Therefore, this research effort proposes PSE approaches to tracking and estimating chemicals of concern across POTWs that foster bottom-up process modeling and chemical allocation to simulate fate and transport comprehensively.

The work introduces a POTW design, modeling, and simulation model that integrates detailed representation

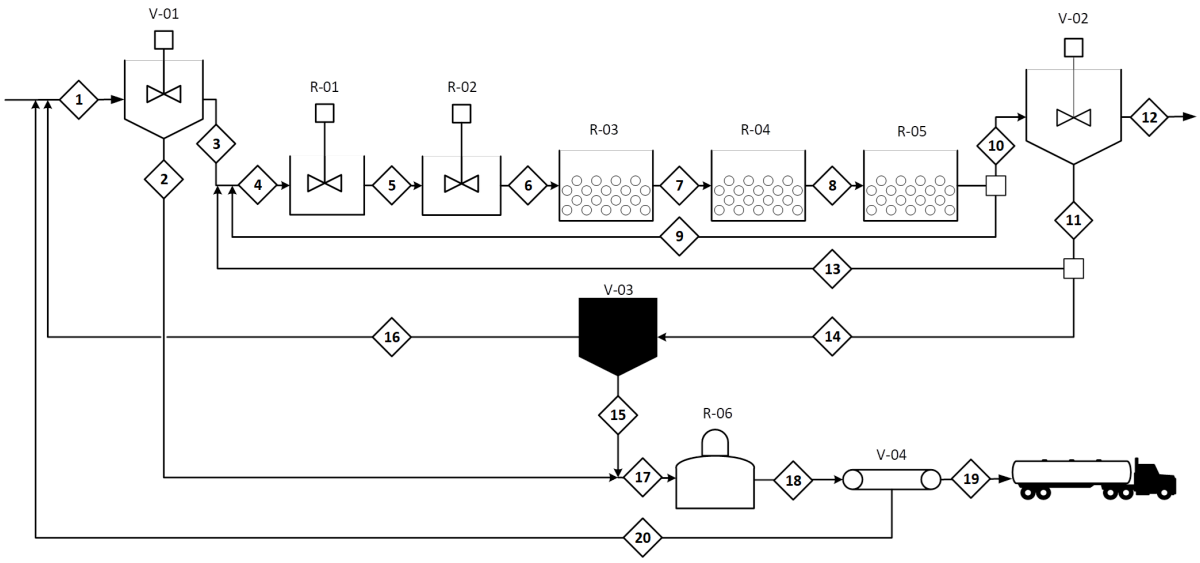


Figure 3. A process flow diagram of a generic publicly owned treatment works (POTWs) vessels(V-0X) and reactors(R-0X). Process units include a primary clarifier (V-01), a secondary clarification unit (V-02), a sludge thickening unit (V-03), a dewatering unit (V-04), aerated and unaerated activated sludge unit (R-01;R-05), and anaerobic digestion equipment (R-06)

Table 1. Methylene Chloride mass flows across streams #1 to #20 describing fate and transport

Stream	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Flow Rate (m^3/d)	21096	148	20948	103201	103203	103203	103203	103203	61922	41281
Mass Flow-CH_2Cl_2 (kg/d) in Various Phases										
Liquid	104	0.7	102	112	111	110	74	49	20	13
Solid	3	1	1	24	24	24	16	10	4	3

Stream	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**
Flow Rate (m^3/d)	20641	20641	20331	310	31	279	179	179	10	169
Mass Flow-CH_2Cl_2 (kg/d) in Various Phases										
Liquid	6.5	6.3	6.4	0.1	.01	0.1	0.6	0.4	.02	0.3
Solid	3	.003	3	.04	.04	.001	1.2	0.2	0.2	.004

of individual process units from primary clarification to advanced biological treatment, delineating settling characteristics, biological transformations, nutrient removal, and sludge management. Process units include a primary clarifier, a secondary clarification unit, an aerated and unaerated activated sludge unit, an anaerobic digestion equipment, and an influent generator model that creates influent profiles mimicking POTW influent variations as illustrated in **Figure 3**. The model captures interactions between chemicals of concern and wastewater treatment operations, allowing for the estimation of chemical partitioning across unit operations such as sedimentation, biological treatment, adsorption, volatilization, and transport mechanisms. The selection of volatile organic compounds (VOC) as the first chemical class for model integration stems from their distinct behavior within the proposed treatment processes, characterized by their volatility, sorption, and biological uptake tendencies.

Table 1 shows the mass flow changes and notable reductions to solid and liquid phase methylene chloride (CH_2Cl_2) from influent to effluent, showcasing removal rates at each process unit. The substantial reduction in CH_2Cl_2 concentrations, primarily attributed to biological degradation mechanisms within secondary treatment (stream # 4-10), along with the lack of adsorption capacity seen throughout the plant, aligns with real-world scenarios [15].

Our proposed PSE-based approach, employing bottom-up methodologies, offers a valuable tool for assessing the efficiency of different treatment strategies and showing potential areas for improvement in EoL chemical management. The usability and value of this model extend to its potential applications in environmental risk assessment, regulatory compliance, and the development of more effective treatment methodologies.

CONCLUSIONS

This work describes a computational framework based on data engineering, data-driven modeling and PSE models to predict EoL chemical releases and potential occupational exposure scenarios. This contribution also shows a comprehensive EoL database created from publicly accessible domestic and international regulatory systems. Moreover, this contribution describes the application of GREENSCOPE to inform the development of more sustainable chemicals by reducing their environmental and human health impacts, implementing pollution prevention, and source reduction while increasing economic and social benefits. This multi-stakeholder analysis can be extended toward potential trade-off analysis, such as trading costs, the highest-performing category, investing in recovery processes, better waste treatment and management procedures, and selecting renewable materials sources for manufacturing. The gradual adoption of material management and selection guidelines and process improvement opportunities can allow EoL chemical generators to take on a more active role in aiding the shift of linear economy practices toward the state of a circular economy.

Future steps are to understand the near-field exposure associated with circular economy paths and compare the composition and functionality between recycled and brand-new products to avoid unintended recycling of toxic substances at post-recycling/recovery activities, including chemicals not currently subject to USEPA regulatory programs. To resolve this problem, we can use data engineering and data-driven approaches to effectively combine facility, PAU, and equipment level data. This integration would enable the detection of potential EoL exposure scenarios, calculation of releases, and monitoring of upstream recycling scenarios for chemicals of concern. The CFA will utilize PAU/equipment-level data to estimate releases inside chemical facilities and allocate chemicals into environmental compartments. Facility-level data will provide insights on regulatory affairs, as well as the behavior of the supply chain and interconnectivity of chemicals in the EoL stage of the industry. Future research should concentrate on integrating isolated environmental regulatory data and developing modeling pipelines and architecture. These can range from graph representation learning for supply chain simulation to hybrid modeling for combining top-down (chemical facility data and models) and bottom-up (operating units, equipment)approaches.

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