



## Data engineering - solution for the lifetime of chemical compounds.

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**Abstract.** Every year, mankind and the environment are exposed to chemicals. Numerous chemicals may present a risk to health or the environment during production, processing, distribution in commerce, use or end of use. Through data engineering it is possible to trace chemicals, estimate emissions and identify possible exposure scenarios for the different chemical compounds at the end of life of the industrial processes involved.

This mini review identified case studies based on food, pharmaceuticals and N-hexane, concluding that data engineering can help to track chemicals in waste streams generated in industrial activities handled in off-site facilities, identifying possible exposure scenarios to a chemical in question.

Every year, mankind and the environment are exposed to chemicals. Numerous chemicals may present a risk to health or the environment during production, processing, distribution in commerce, use or end of use. Therefore, regulations are in place to track and manage chemicals throughout their life cycle. A chemical risk assessment supports the selection of safer profile chemicals and regulatory decision-making to protect human health and the environment. It has been identified that through different databases, a data engineering framework can be developed to track chemicals, estimate emissions and identify possible exposure scenarios in end-of-life streams of different industrial processes. This mini-abstract will present different studies carried out in data engineering, focused on the flow of chemical products and their useful life.

Hernandez et al.,2021, shows that chemical flow analysis allows decision makers to identify potential environmental releases and exposure pathways at the EoL (End-of-Life) stage and therefore improves the estimation of chemical exposure.

This work improves and extends a recently published EoL data engineering framework by using publicly available databases, data-driven modeling and analytical hierarchy approaches to track chemicals, estimate emissions and potential exposure pathways in on-site industrial pollution management operations. The expanded framework develops PAU (Pollution Abatement Unit) technologies and estimates their efficiencies, chemical emissions, exposure media, operating expenses and capital expenditures.

The framework integrates multiple publicly available databases and employs data-driven models and MCDM (Multi-Criteria Decision-Making) to develop PAU technology systems. However, more data collection should be required to reduce the uncertainty of cost data and increase the reliability of data-driven models.

The above was performed in three IS (Industry Sector) based case studies of food and pharmaceuticals illustrating the application of the enhanced and extended framework with the PAU dataset modules. The results show how the enhanced framework designs and evaluates PAU technology systems that handle single and multiple chemicals in EoL streams and provides release inventories and pathways to perform chemical exposure assessments (Hernandez et al., 2021.a,c).

Likewise in other research this author has identified another case study based on n-hexane (CAS 110-54-3) to demonstrate the usefulness of the framework to perform CFA (Chemical Flow Analysis) to trace the chemical along the chemical EoL management chain and close the recycling loop. It should be noted that N-hexane is part of the Organization for Economic Cooperation and Development's list of high production volume chemicals, which are chemicals produced at levels above  $1.00 \times 10.6$  kg/year. (Hernández et al., 2021.b).

## Conclusion

- The results show how data engineering designs and evaluates PAU technology systems that handle single and multiple chemicals in EoL streams and provides release inventories and pathways to perform chemical exposure assessments.
- Data engineering can help track chemicals in waste streams generated in industrial activities and handled at off-site facilities, identifying possible exposure scenarios to a given chemical.

## References

Hernandez-Betancur, J. D.; Martin, M.; Ruiz-Mercado, G. J. A data engineering approach for sustainable chemical end-of-life management. Resources, Conservation and Recycling 2022, 178, 106040.a

Hernandez-Betancur, J. D.; Martin, M.; Ruiz-Mercado, G. J. A data engineering framework for on-site endof-life industrial operations, Cleaner production 2021.b

Hernandez-Betancur, J. D.; Ruiz-Mercado, G. J., Martin, M.; Abraham, J., Smith.R. Data engineering for tracking chemicals and releases at industrial end-of-life activities. Hazardous Materials,2021.c