ISGC 2019
May 13th - 17th

N°453 / OC / PC
TOPIC(s) : Life cycle and environmental assessment / Chemical engineering

How to simplify the assessment of life cycle impacts for new organic reactions? Development of a tool and application to a catalytic reaction.

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PURPOSE OF THE ABSTRACT

Growing concerns regarding the diminishing supply of feedstocks and energetic resources and increasing environmental pollution have led the chemical community to redefine its way of thinking from a yield-focused approach to an enlarged vision directed towards sustainable development. In this context, modern chemistry is developing around the concept of ?Green Chemistry? [1]. Main goals of this approach include atom efficiency, waste prevention, use of less toxic and hazardous chemicals, catalytic rather than stoichiometric processes.
However, the sustainability of these new developments is rarely assessed and it makes it difficult to compare new reactions with alternatives. Since the 90's, simplified metrics such as the E-factor are used to assess the environmental impact of a new reaction [2]. Such metrics are limited because they cannot assess in a holistic way all the environmental impacts arising from the life cycle of the products. To this end, Life Cycle Assessment (LCA) is a normalized and relevant tool that can assess bring such quantitative metrics. Nevertheless, application of LCA to new developments at the lab scale is not trivial because it requires expertise and data that are not necessarily known by the chemist. Also, it is complex to model the impacts of new products at industrial scale.
To tackle these issues, we developed a methodology and an associated tool that enable to assess environmental impacts of new chemical products with data that are easily accessible for the chemist at the lab scale (types of reactants and solvents, yield of the reaction, temperature and duration of the reaction, etc.). From these data, quantity of inputs (reactants, solvents), generation of waste (air emissions and wastewater), and energy use during the reaction at both the lab and industrial scale are quantified. This is done with a set of assumptions and modeling approaches about the nature of chemicals and energies, the question of recovery and treatment of them by distillation, incineration and waste water treatment adapted for the fine chemical industry[3]. It results in precise life cycle inventory foreground data that can be included in SimaPro software using the ecoinvent database for background data to compute life cycle impacts.
This procedure has been tested for comparing different catalytic systems for the aldol reaction metal catalyst, organo-catalyst, and enzyme [4]. Input data at the lab scale were collected from the chemistry literature. It shows that for all reactions, solvent production as well as waste treatment (through distillation/incineration or waste water treatment) has an important contribution to impacts. Modelled impacts at the industrial scale are therefore sensitive to the quantity of solvents used and to the fate of the waste and co-products. It is also possible to compare the catalytic reactions at both the lab scale and at the industrial scale considering different assumptions regarding quantity of solvents used, recovery rates by distillation, etc.
This study shows that LCA can inform chemists on the environmentally friendly of their catalytic systems with quantitative values and brings information to eco-design the reactions. As a perspective, the developed methodology has the ambition to bring to chemist a simplified ready-to-use eco-design tool.

FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

Life Cycle and Environmental Assessment | Catalysis | Chemical Engineering

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