IMPROVED CHARACTERIZATION OF DETERGENT (ECO)TOXICITY IN LCIA USING REACH EXPERIENCE

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ABSTRACT

Life Cycle Assessments of three detergents products from Chemolux-McBride group are analysed in order to evaluate the environmental improvements provided by the novel formulations. Detailed discussion of the characterization factors (CFs) developed within the USEtox model for freshwater ecotoxicity and human toxicity is provided. In particular, the publicly available data collected under REACH were used for the development of the CFs. The results demonstrate the benefit of removing phosphate ingredients. Several limitations in the CF development process were found: for example the endpoints required by the REACH regulation are different from the ones required by USEtox. Nevertheless, the two approaches can be used to obtain harmonized and complementary results.

INTRODUCTION

The composition of dishwasher detergents is highly regulated and the European Union Member States agreed to ban phosphorous as ingredient due to the eutrophication potential. According to the literature review, several studies focused on laundry detergent products, evaluating the environmental performances of different formulations using the Life Cycle Assessment (LCA) methodology (ISO 1040 and 14044, 2006). These studies had a special focus on freshwater ecotoxicity potential of the effluent from dishwasher. However, the chemicals included in the effluent, mainly coning from the detergents composition, are hardly characterized by the current Life Cycle Impact Assessment (LCIA) methods and therefore new characterization factors need to be developed, for example using the USEtox model (Rosenbaum et al., 2008), as in Van Hoof et al. (2011).

In this paper, the LCIA results of three detergents products from Chemolux-McBride group are analysed in order to evaluate the environmental improvements provided by the recent novel formulations. Detailed discussion of the characterization factors (CFs) developed within the USEtox model for freshwater ecotoxicity and human toxicity is provided. In particular, the publicly available data collected under REACH (European Commission, 2006) were used for the development of the CFs, taking profit from the links between REACH and LCA (Askham, 2012). Comparison with existing results from literature as well as sensitivity analysis have been performed to highlight the robustness and limitations of the results.
MATERIALS AND METHODS

A phosphate-based tablet (PB), an eco-labelled tablet (EL) and a phosphate-free soluble bag (PF) were analysed. For each detergent product, the life cycle inventory is based on the use of the detergent product, using formulation data from the producer and removal performances of wastewater treatment plant (treating the effluent) from literature. Freshwater ecotoxicity and human toxicity have been characterized for the effluent after one washing cycle and a partial removal in the wastewater treatment plant. Regarding the three detergents, only four ingredients in total were already characterized by USEtox. New CFs have been developed for the other substances, assuming a cut-off of 1%, in order to focus on the main substances. Polymer compounds were modelled considering acrylic acid as a proxy due to the general lack of data on polymers. Nine other substances were specifically characterized: alcohols C11 ethoxylated propoxylated (AE C11), alcohols C8-C10 ethoxylated (AE C8-10), disodium carbonate compound with hydrogen peroxide (Na-percarbonate), N,N'-ethylenebis[N-acetylacetamide] (TAED), pentasodium triphosphate (STP), polyethylene glycol (PEG), silicic acid sodium salt (Na-silicate), sodium carbonate (Na-carbonate) and tetrasodium (1-hydroxyethylidene) bisphosphonate (4Na HEDP).

The USEtox model describes the cause-effect chain of a chemical emitted into the environment: fate, exposure and effect. The CF is obtained by multiplying these three factors. For freshwater ecotoxicity, the unit is PAF.m².day.kg⁻¹ (PAF for Potentially Affected Fraction of species), while human toxicity is expressed in cases.kg⁻¹. New CFs can be calculated using an Excel sheet provided by the USEtox developers.

In USETox, the fate of the substances in the environment is based on a multimedia model, requiring twelve physicochemical parameters which can be reduced to eight in case of organic substances under specific assumptions. For the four inorganic substances contained in the studied detergents, (Na-percarbonate, STP, Na-carbonate and Na-silicate), the same eight parameters were also considered by default, due to a lack of data. The specific parameters proper to each substance were retrieved from EPI Suite™ model (2013) if no experimental data were available in the HERA reports (2013). No data were available for Na-percarbonate: properties similar than the ones of Na-carbonate and Na-silicate were assumed and no degradation potential (as in Van Hoof et al., 2011). Environmental exposure is calculated through the dissolved fraction in freshwater, while human exposure is evaluated via the potential transfer pathways (water drinking, air inhalation, food ingestion, etc.).

The effect of the pollutant is assessed through: i) its ecotoxicity potential, based on the geometric mean of chronic EC50s, i.e. the effect concentration at which 50% of the tested population are affected; and ii) its toxicity potential, based on chronic ED50, i.e. the effect dose which affects 50% of the tested population. These toxicity endpoints were mainly collected from the ECHA portal (2013) as data are up-to-date and presumably complete. In case of missing data, other databases were used (OECD eChem, PAN Database, ChemID or ECOSAR from EPI Suite™). In some cases, extrapolation factors defined in USEtox were applied in order to account for different time of exposure (e.g. factor of 2 between acute and chronic EC50s), interspecies differences (e.g. factor of 4.1 between rat and human ED50s) or endpoint differences (e.g. factor of 9 between NOAEL and ED50). Furthermore, there is no indication that the assessed substances are carcinogenic and only non-carcinogenic effects to humans were therefore evaluated.
**RESULTS**

CFs for freshwater ecotoxicity were calculated for the nine substances while only four CFs could be developed for human toxicity (AE C8-10, TAED, Na-silicate and 4Na HEDP) due to lack of repeated doses tests in the toxicity databases. After integration of these newly calculated values, the USEtox results for the effluents from the three detergents are presented in Figure 1. More than 95% of the effluent composition is characterized for freshwater toxicity whereas only less than 40% is represented for human toxicity. Regarding the three detergents, the main contributing substances are Na-carbonate, Na-percarbonate, acrylic acid (proxy for all polymers), Na-silicate and STP. The large contribution of STP in the PB product highlights the benefit of its removal into the new formulations (EL and PF). When assessing the freshwater ecotoxicity of the overall lifecycle of the detergents, the effluent contribution varies from 60% to 80% of the whole lifecycle impact. This result emphasizes the importance of the characterisation of the effluent composition.

![Figure 1: Comparison of a) freshwater ecotoxicity and b) human toxicity (without carcinogenic effects) of the effluent from EL, PF and PB detergents.](image)

**DISCUSSION**

A comparison between the developed CFs and the ones of Van Hoof et al. (2011) was carried out for eight substances which were in common. The resulting variation of CFs is acceptable (same order or one order of magnitude difference). The differences show, however, the sensitivity of the USEtox model with respect to the data source and to the practitioner choices. Sensitivity analysis was also carried out on each parameter of the model. The ecotoxicity effect was found to be the most influencing one. Results for fate properties were only sensitive to the degradation rate in water, in accordance to Birkved and Heijungs (2011).

The development of CFs within USEtox model implies several limitations. First, the fate model is hardly applicable to inorganic compounds. In order to improve their assessment, the potential organic dissociation products could be studied. Evaluating the impact of the mother compound can lead to overestimations because only part of the dissociation products could be toxic. Secondly, the effect assessment suffers from a lack of available data, in particular if the chemical has not yet been registered under REACh. Even in the case of a registered substance, the chronic EC50 and ED50 endpoints required by USEtox are rarely reported
because other endpoints are used in the regulatory assessment and partially or no reliable data are provided in the registration. The lack of availability and/or reliability of data can lead to the use of extrapolation factors increasing the uncertainty of the assessment.

**CONCLUSIONS**

The results confirmed the environmental benefits of removing phosphate ingredients from the composition of dishwasher detergents. The importance of characterizing new substances was proven by the high contribution of the effluent to the overall ecotoxicity of the detergents lifecycle. For a more consistent comparison of the products, other environmental categories should also be considered. The present work focused on the development of CFs within USEtox to characterize only the (eco)toxicity of the detergent ingredients. The comparison with previous studies showed that the model was quite stable. The most sensitive parameter is the effect factor, which requires therefore special attention by the practitioners. The endpoints have been selected using data collected under the REACH regulation. Although the two frameworks are fundamentally different, they can benefit from each other to increase data availability and reliability, as well as provide harmonized results to the industry.

**REFERENCES**


