A model and tool to calculate life cycle inventories of chemicals discharged down the drain

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1. Introduction

A new model and tool to calculate life cycle inventories (LCIs) of chemicals discharged down the drain is presented, which includes treatment in a modern municipal wastewater treatment plant (WWTP), sludge disposal, as well as the greenhouse-gas (GHG) and nutrient (N, P) emissions occurring from direct discharges in the environment. The main innovation of this model is its completeness and the fact that it attributes the exchanges with the technosphere and the environment taking into account the expected behaviour of individual chemicals in the WWTP and the environment. This contributes to better decision making and data availability in the context of the life cycle of chemicals.

2. Materials and methods

Figure 1 shows an overview of the model's concept. A chemical substance's properties are used to predict its fate in a WWTP, as well as in the environment. Based on the predicted fate factors, the model calculates an LCI including the operation of the WWTP and sludge disposal processes (landfilling, incineration, agricultural use), as well as emissions from degradation in the environment of any fraction of the chemical directly released to the environment. The model is programmed in an Excel spreadsheet, the WW LCI tool, which contains all the elements in the white boxes shown in Figure 1. The current implementation in Excel accommodates simultaneous calculations for 30 chemicals, individually or as a mixture.

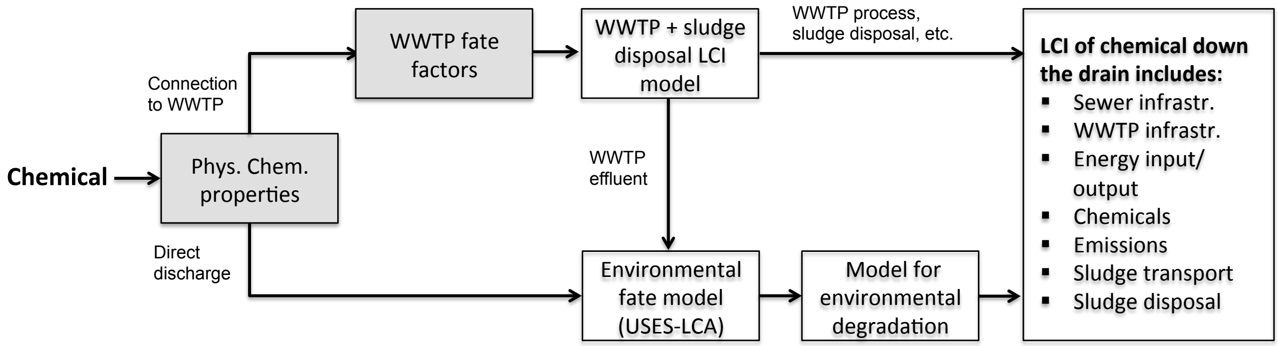

Figure 1. Conceptual diagram of the WW LCI tool.

The model covers the treatment of organic as well as inorganic chemicals. Input variables by the user include:

- **Chemical-specific variables**: definition as organic/inorganic, composition in terms of C, H, O, N, S, P, Cl, carbon origin (biogenic/fossil), anaerobic degradability (yes/no), generic physical-chemical properties (molecular weight, vapour pressure, solubility, Kow, etc.), half-lives in the environment, and fate factors in the WWTP (F_{air}, F_{sludge}, F_{deg}), namely the fraction of chemical mass expected to partition to air, to sludge, or to degrade in the WWTP, respectively.
- **Scenario variables**: Percentage of population connected to WWTP, country, biological N removal in WWTP (yes/no), chemical P removal in WWTP (yes/no), percentage dry matter in dewatered sludge, percentage of sludge disposal by landfilling, incineration, landfarming.

The WWTP is modelled by means of a mass and energy balance that takes into account the partitioning of the chemical to air, sludge, treated effluent, and depending on its degradability, the transformation by microorganisms to CO_2 and new biomass (excess sludge). Sludge is treated by means of anaerobic digestion and biogas is burned for energy recovery.

The fate of any fraction of chemical released to the environment (e.g. treated effluent, direct discharges) is assessed with the model developed by Muñoz et al. (2013), which calculates GHG emissions following degradation in environmental compartments (air, water, sediments). Besides GHG emissions, emissions of nutrients (N, P) are also considered.

Sludge disposal by incineration and landfilling is assessed by means of the models developed by Doka (2007), whereas reuse of sludge in agriculture is accounted for by means of a specific set of calculations using emission factors, mainly from IPCC (2006).

Overall, All exchanges between the system and the environment and the technosphere are calculated based on the chemical's composition and expected behaviour, thus following a cause-effect relationship.

3. Results and discussion

The output of the WW LCI tool is a comprehensive inventory (Figure 2, left) linked to ecoinvent v3 data sets, that can be imported to LCA software in order to complement a life cycle assessment study of a particular chemical or a chemical mixture associated to a product or service. Impact assessment calculations are then easy to perform for different impact categories, such as carbon footprints (Figure 2, right), eutrophication and freshwater ecotoxicity, among others.

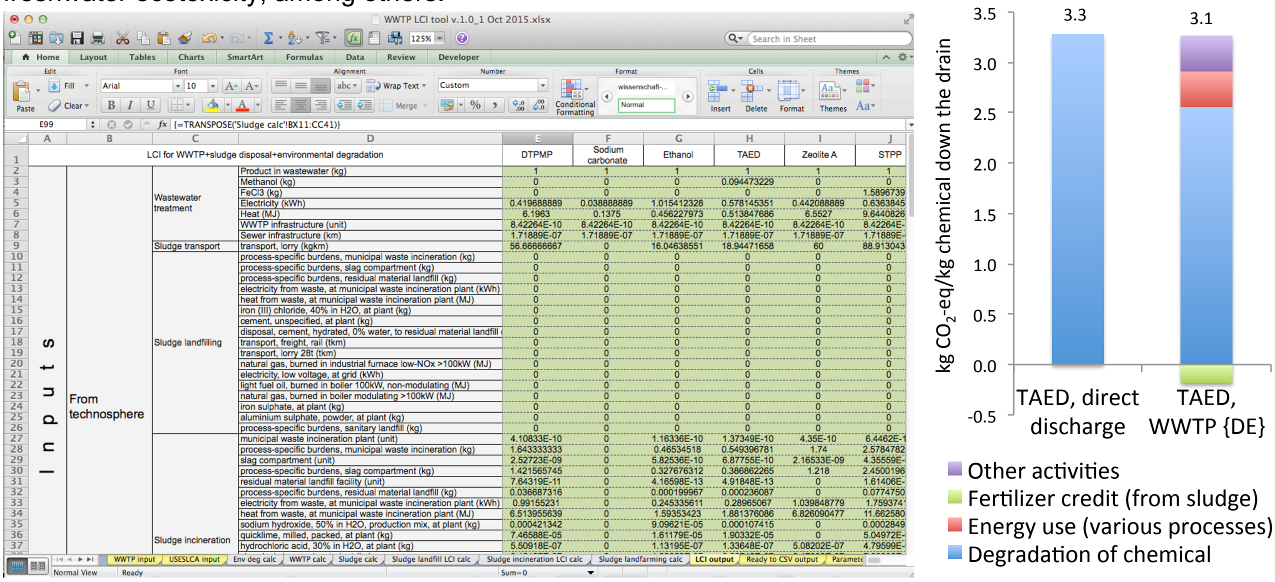

Figure 2. Left: Screenshot of the WW LCI tool showing part of the LCI output tab. Right: GHG emissions per kg tetraacetylethylenediamine (TAED) discharged down the drain in two scenarios: direct discharge (0% connection to WWTP) and Germany (100% connection to WWTP). Impact assessment calculations carried out in the software SimaPro 8.0.4 with global warming potential (GWP) for a time horizon of 100 years.

4. Conclusions

This model is the first one to address a chemical-specific and comprehensive LCI of chemicals discharged down the drain, including not only treatment in the WWTP but also sludge disposal and degradation of chemicals in the environment when there is no connection to a WWTP. This is particularly important since emissions from direct discharges can be important (Muñoz et al. 2013). This model constitutes an advance over previous WWTP models using generic descriptors like BOD, COD, etc. and despite its limitations and room for improvement, it constitutes an advance in how the end-of-life stage of chemicals is addressed in LCA.

5. References

[1] Muñoz I, Rigarlsford G, Milà i Canals L, King H (2013) Accounting for greenhouse-gas emissions from the degradation of chemicals in the environment. Int J Life Cycle Assess, 18 (1): 252-262.

[2] Doka, G. (2007) Life Cycle Inventories of Waste Treatment Services. Final report ecoinvent 2000 No. 13, EMPA St. Gallen, Swiss Centre for Life Cycle Inventories, Duebendorf, Switzerland.

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