Screening organic chemicals in commerce for emissions

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Background and objectives

Significant efforts are carried out to identify organic chemicals which may represent a hazard to the environment, based on individual attributes such as persistence, bioaccumulation, toxicity and long-range transport potential – or combinations thereof[1-3]. However, potential risks to wildlife and humans from chemical exposures are also a function of actual emissions. The objective of this study is to develop methods for estimating "expected" regional scale emission rate and mode-of-entry to support risk-based exposure modelling efforts[4] [see also ECO3P WE 026 Poster by Arnot et al.]. The modelling hypotheses of "expected" concentrations in the environment will be subsequently tested by measuring environmental samples.

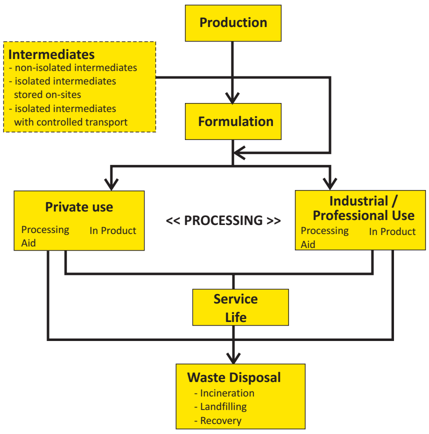

Figure 1. Life-cycle of a substance (from EU TGD)5.

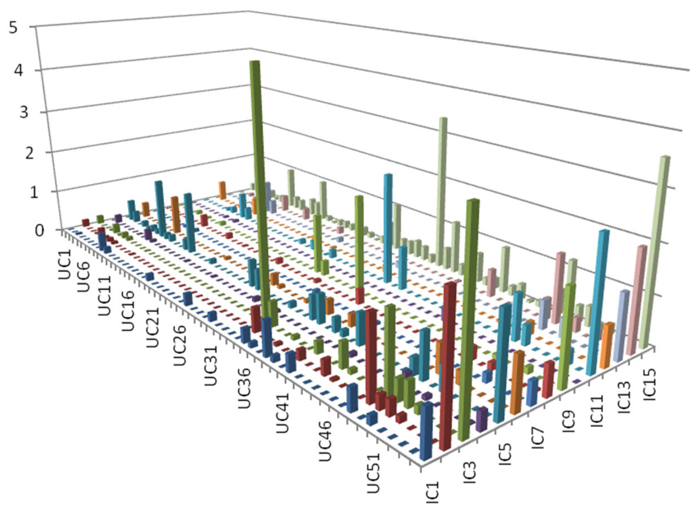

Figure 2. IC/UC combinations reported for EU HPV substances (in %).

Methods

Organic substances on various high production volume (HPV) lists within Europe, Japan, USA, Canada or OECD were considered[2]. Emission scenarios were calculated on the basis of the EU TGD[5] (Fig. 1). In brief, emissions to air, soil and water are calculated for each main stage of the life-cycle using information on both physical/chemical properties and industrial and use categories (IC/UC) as input. While the physical/chemical properties can be estimated[2-3], the IC/UC information is frequently difficult to obtain.

Results and discussion

- The frequency of occurrence of different combinations of IC and UC was obtained from non-confidential European HPV data (N=~2800 chemicals) to obtain a default frequency distribution for 248 plausible IC/UC combinations (Fig. 2).
- Up to 248 emission scenarios were derived for each chemical, dependent on the availability of information on ICs/UCs (Fig. 3).

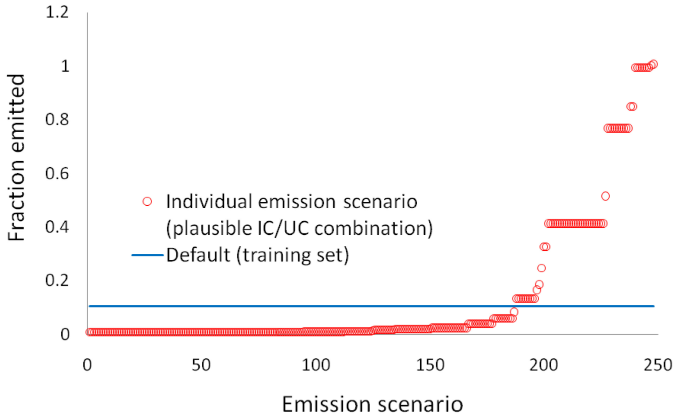

Figure 3. Fraction of overall production emitted to the environment over the entire life-cycle for a given substance with no available information on IC/UC.

In the absence thereof, the 248 emission scenarios were weighted against the frequency distribution in Fig. 2.

- The overall results are shown for ~13,000 substances, using emissions to air as an example (Fig 4). Min/max values were calculated from the min/max overall production and the emission scenario with the lowest/highest emissions.
- Confidentiality issues create difficulties in estimating emissions and hence in identifying potential unknown PBTs and POPs among existing chemicals in commerce. However, order of magnitude estimates will help discriminating between chemicals which should be of no concern and worrisome substances which require further scrutiny.
- Back-calculating critical or threshold emissions using the RAIDAR model[4] may be a further way to focus priorities on refined emission rates for more worrisome chemicals.

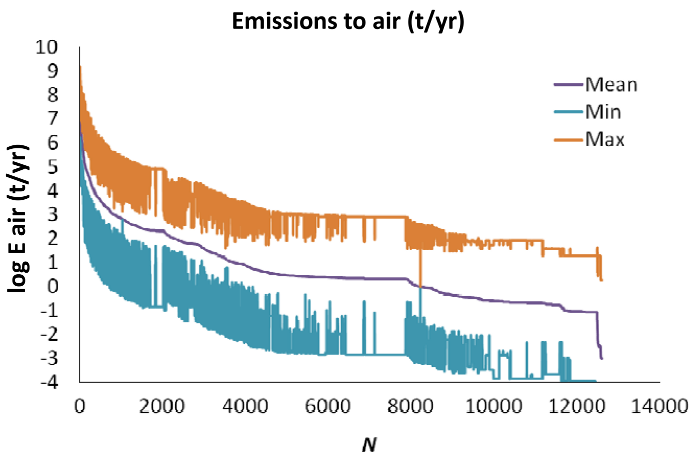

Figure 4. Estimated emissions to air over the entire life-cycle (ranked from high to low).

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References

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