

Chemicals in statistics – a source for information on environmentally relevant compounds?



Tomas Öberg^{1,*} and Louise Sörme²

¹ School of Pure and Applied Natural Sciences, University of Kalmar

² Statistics Sweden, Environmental Accounts

*E-mail: tomas.oberg@hik.se

Introduction

The success in reducing pollution and emissions of chemicals to the environment can be followed by monitoring programs and statistics regarding the use of specific chemicals.

Yet another source of information is the official trade and manufacture statistics based on the Combined nomenclature eight digit codes (CN) of the European Union for groupings of chemicals.

Each CN code for chemicals is linked to a number of Chemical Abstract (CAS) registry numbers, which provides unique identifiers for the specific compound in question.

The net use of chemicals can be assumed to provide an indication of potential emissions. Specific chemicals, nevertheless, differ substantially in properties and effects. Summation of turnover for all chemicals does therefore not provide the information needed, to indicate the direction of development with regard to the environmental objectives.

It was recently suggested to use the ratio of the atmospheric persistence (half-lives) to the baseline toxicity – expressed as median lethal concentrations (in water) (LC_{50}) – to provide a continuous scale to rank and summarize the incremental environmental impacts from the simultaneous exposure to many chemicals [1]. The toxic persistence rating (TPR) is expressed as:

$$TPR = \frac{\text{Atmospheric half - life (days)}}{LC_{50} \text{ (mg L}^{-1}\text{)}}$$

Two validated structure-activity relationships (SAR), for baseline toxicity and hydroxyl radical reaction rate constant, form the basis for these calculations [2-3].

The purpose of this investigation is to evaluate the use of trade statistics and the suggested toxic persistence rating to screen for chemical groupings of particular interest [4].

Materials and Methods

Baseline toxicity, atmospheric persistence and the resulting toxic persistence ratings (TPR) have previously been estimated for a database of 50 000+ compounds using SAR models [1].

This database was matched against 28 504 CAS registry numbers corresponding to CN codes from the ECICS database and both the SAR models for toxicity and persistence were then applicable for 10 578 compounds. However, most CN codes represent a range of chemicals (sometimes more than 100).

Results and Discussion

The 10 578 compounds with matching TPR-estimates were ranked and the top 100 selected for further study.

The selected compound groups represent a variety of chemicals, but 95% of them are halogenated. The two largest groups were halogenated aromatic compounds (25) and HCFCs (20).

The net use of chemicals (import and domestic production minus export) for these two groups can be followed in the trade statistics, table 1.

Table 1: Import and export (metric tons).

Year	Halogenated aromatics		HCFCs	
	Import	Export	Import	Export
1998	110	0.2	360	170
1999	11	2.5	190	210
2000	12	1.1	100	270
2001	11	0.007	17	190
2002	3.1	0.05	28	75
2003	23	11	4.5	190
2004	67	0.3	24	190
2005	48	0.2	18	210

Two observations can be made from this table:

- The import of halogenated aromatic compounds has not decreased
- The export of HCFCs is substantially higher than the import

A comparison with the Products Register of the Swedish Chemicals Agency supplied contradictory information. The import of halogenated aromatics seems to have declined below 1 metric ton. Commercial secrecy, however, prevents the disclosure of any export figures.

Re-export to final treatment (destruction) outside Sweden could be a possible explanation for the high export of HCFCs.

Conclusions

The self-reported statistics seem to need further validation to improve its usability for evaluating the accomplishment of the environmental objectives concerning chemicals.

The two data sources, foreign trade statistics and the Products Register, offer an excellent opportunity for validation studies by joining the data bases.

For compounds and compound groups of particular environmental relevance it is also necessary to trace the statistics back to the primary source to clarify possible reporting errors. Further analysis of the CN codes with assumed PBT properties is recommended.

A more detailed study of the net chemical use expressed in TPR-units can be achieved by directly linking the TPR-estimates to the net use for individual compounds (from the Products Register).

Acknowledgement

We like to thank the following persons for valuable help and comments to the work: Viveka Palm, Christian Surtin and Anders Wadeskog, Statistics Sweden, Margareta Östman, Åsa Almqvist and Carl-Henrik Eriksson, Swedish Chemicals Agency and Maria Ujfalusi, Swedish Environmental Protection Agency.

References

1. Öberg, T. (2004). A QSAR for baseline toxicity: Validation, domain of application, and prediction. *Chemical Research in Toxicology* **17**, 1630-1637.
2. Öberg, T. (2005). A QSAR for the hydroxyl radical reaction rate constant: Validation, domain of application, and prediction. *Atmospheric Environment* **39**, 2189-2200.
3. Öberg, T. (2006). Virtual screening for environmental pollutants: Structure-activity relationships applied to a database of industrial chemicals. *Environmental Toxicology and Chemistry* **25**, 1178-1183.
4. Öberg, T. (2009). *Chemicals in Statistics - Method Development*. Background facts Regional and Environment Statistics 2009:4. Statistics Sweden.