Towards a screening procedure for identification of representative case-studies describing the economy-wide emissions of chemical substances from articles during their life-cycle

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Introduction

Industrial production of chemicals constitutes a huge mass-flow that provide for an extensive consumer use of chemical products and chemical substances as constituents of articles, giving benefits of various kinds, ranging from basic needs to luxury elegance. The downside of the giant flow is the emissions of a very wide range of substances that expose humans and the environment causing a set of known, and unknown, risks for unwanted deleterious effects. Coming to grips with the very many diffuse emissions of chemical substances from the technosphere include more than the identification of possible point sources during production of chemicals and goods. Also the diffuse emissions of substances occurring during the different life-cycle stages of products need to be covered in the description. Much research has been done on identification and quantification of emissions, distribution, fate and effects of chemicals, particularly on chemical substances known to pose specific risks (such as pesticides) but there is still a great lack of knowledge about emissions of very many common chemicals, and no objective method exist in order to estimate the relative importance of substances with regard to emissions from the technosphere, and whether it is point sources or diffuse emissions from end-use and waste handling that are the main sources.
Attempting at an answer to the question of the relative importance of substances and sources we here briefly describe a method to identify relevant and representative substances of concern, occurring in significant amounts in products, which are used under a particular set of conditions resulting in potentially significant emissions to the environment. We thus take the combination of the concepts "chemical substance", "product" and its "use" as starting points for a screening method intended to identify a small number of specific products, with a significant use, which contain chemical substances of concern from an environmental emissions point of view that lead to emission worth to consider.

Aim and scope of report

This very brief report aims to give only an overview of the basic steps performed to identify the cases. The details of the different steps are therefore not covered in detail.

Aim and scope of screening procedure

The aim of the procedure, which is part of a larger reserch program called Chemitecs (funded by Swedish EPA), was to identify 6 to 10 products that during the intended use release a significant amount of a chemical substance of environmental concern.
The scope included organic substances emitted from "articles" (a term inspired by the REACH legislation) but excluded chemical products, cosmetics, pharmaceuticals, biocides, food, and food packaging material. All these product categories are outside the scope of the REACH-legislation.

Identification of substances of concern

The identification of substanced followed an objective method based on criteria related to production volume and substance properties. Initially, the chemicals on the European Chemicals Bureau (ECB) lists of high production volume chemicals (HPVC) and low production volume chemicals (LPVC) and a selection of chemicals that are commonly used as additives in the plastic, rubber and textile industry were included. Chemicals produced or imported in volumes less than 10 tonnes per year were excluded. This list was then complemented with a number of chemicals

identified as being hazardous or potentially hazardous in other studies so that the total list consisted of almost 10000 compounds. After elimination of inorganic compounds, ill-defined mixtures, and polymers (that are considered too non-volatile and insoluble to be emitted) about 7000 compounds remained.
All compounds were then further characterized by calculated molecular attributes selected to cover interesting chemical properties, which for this project means properties describing (or indicating) emission tendency, long range transport and different types of biodegradation and bioaccumulation descriptors. Chemicals of concern are those that are easily emitted from products and at the same time have properties that enable them to persist and accumulate in the environment. The selection strategies can be seen as filters, where the substances are filtered with regards to important environmental and emission related aspects (e.g. LRT, PBT, volatility). By using multivariate characterization (PCA) in combination with the different property filters and statistical design, sets of case object chemicals were selected. The chemical selection strategy is described in more detail in the recently accepted publication by Rännar and Andersson (J Chemical Information and Modeling).

Identification of products

As an important input to the process of identifying product categories to focus, the national trade statistics was employed. The statistics rely on an international nomenclature, the so called combined nomenclature (CN), that cover all traded goods and consists of 98 chapters with at least 12 000 statistical categories. The CN is roughly organised as a generalised value-chain where raw materials are found in the first chapters (ore, metals) and the complex end products (e.g. cars) are found at the end. Furthermore the CN-categories are hierarchically organised making very detailed descriptions of categories possible. However, the actual statistical data in the CN-tables often only pertain to less detailed categories.
After exclusion of CN-chapters considered out of the scope (e.g. chemical products, etc., see above) a set of criteria were applied on the remaining categories in order to bring down the number of CN-categories.
The appraisal of the CN-categories was an iterative exclusion procedure where both objective (e.g. volume) and subjective (e.g. assumed chemical content, availability, and use aspects) criteria were employed by the researchers. The resulting 10 CN-chapters were then subject to a further analysis of use aspects in order to identify a small set of specific products.

Identification of significant uses

The concept of "use aspects" is in this context focused on three factors, that all where estimated using a ranking scheme approach. The three factors included the "stock", the "emission type" and "population exposure".
The ranked values of stock were based on the estimated annually produced volume and a "guesstimated" longevity of the product category. The considered "emission types" contained only two categories, one for molecular emissions and another for cases where particulate emissions are expected to occur (e.g. from abrasion, wear-and-tear etc.). For the second category the total emission is anticipated to be higher due to a much larger surface to volume ration (the surface area is one of the most significant physical factors determining the total emission of a particular compound). The third factor, the population exposure, is estimating the number of persons exposed and the time they are exposed giving a product that represents the population exposure.
Based on this method the CN-categories (about 2500) in the 10 CN-chapters were assessed and 44 specific product categories were identified. To link up these 44 product categories to the

identified chemicals of concern – and thereby closing the loop – detailed knowledge of chemicals content of the specific product categories were needed. This knowledge reside by producers and therefore it was necessary to rely on contacts with industry for the finalization of the identification.

Stakeholder interactions

Using industrial contacts of the research group and by involving the established stakeholder group of the research program it was possible to both get a sufficent input of knowledge regarding the chemicals content of the suggested product categories and inputs related to the feasibility of getting further details of the products, and the relevancy of the particular combination of chemicals, product and use. During the selection procedure two larger workshops were organized with the stakeholder group (including 40 to 50 participants). This work made it possible to bring down the 44 suggested products to 8.

The identified examples

The following 8 cases were finally identified
1 Diisononylphthalate in PVC-flooring.
2. Accelerators (a benzothiazol or benzenediamine) in car tyres.
3. An organophosphate in a LCD-screen.
4. A fluorinated compound used in surface-treated textiles of a car seat.
5. UV-stabilizer (a benzotriazole) in a coated textile.
6. An organotin compound in a piece of furniture.
7. A compound found in concrete (the specific substance not yet defined)
8. A set of substances found in sports shoes.