ChEmiTecs

ChEmiTecs System Boundaries and Delimitations for Dimensioning Study

Johan Tivander

Sverker Molander

Environmental Systems Analysis

Chalmers University of Technology

working document, January 2010

Chemitecs report P1-D6

IVL Svenska Miljöinstitutet · Stockholms universitet · KTH · Umeå Universitet · CHALMERS

1 System boundaries and delimitations - problem dimensioning: what is compared with what?

A main issue in the Chemitecs program is the dimensioning of the problem with emissions of organic chemicals from products. This dimensioning is not possible without a reference and must therefore be done by a comparison(s). The question elaborated on in this chapter is precisely "what to compare?" The environmental problems caused by emissions of organic substances from "products" need to be compared with something, either as an "internal comparison" between different types of products, between different chemicals or with problems caused by something else.

In order to enable such a comparison it is essential to define the system boundaries for "emissions of organic chemicals from products" that separates this system from other causes of environmental problems. Due to the complexity of the product use system and known data gaps, assumptions and delimitations are necessary in order to make quantification possible. Finding quantitative data covering the nation-wide scope, with limited resources available for the study is a challenge. A number of dimensions must be considered both for system boundaries and delimitations. Below is a discussion of these boundaries and a specification of scope and delimitations as far as they have been determined to this point in the program, which comprise the initial emission assessment performed during spring 2010.
Further specifications of the scope of the program will be done iteratively along with findings from the practical work in case studies and from assessing selected product categories.

1.1 Geographical coverage

The emissions due to use of products within the geographical boundaries of Sweden are included in the study. This includes products manufactured in Sweden as well as imported into Sweden. We are well aware that emissions from processes outside Sweden occur. In a first approximation they are not considered, later an inclusion, based on extrapolation of data, might be done.

A portion of all products are transferred over the national boundary which is not accounted for in national toll statistics. This includes private import and export, and illegal smuggling. These products flows are excluded from the study.

1.1.1 We suggest that

- only emissions and environmental concentrations are quantified for emissions occurring in and for environmental compartments of Sweden

1.1.2 This imply that

- no emissions and environmental concentration outside Sweden is covered (even if production and use occurs outside Sweden)

1.2 Temporal coverage

The emissions from the total amount of existing products during one year are included in the study. The exact year represented by the study is to be determined depending on the available data; a typical year within the range from 2000 to 2008 is a first rough temporal scope. Also depending on data coverage it may be possible to produce trends over more than one year.

The accumulation of products into the technosphere is an important aspect. The products produced or imported that year is only a fraction of the total products that exist the particular year. Depending on the maturity of the market for a particular product category and changes in demand the accumulated stock may be rapidly changing between different years. During a given year some products are also leaving the technosphere. Recycling and waste handling are included in the end-of-life stage which needs to be covered. In a first approximation a steady state is assumed in the stock for all products which, in fact, is only most accurate for mature markets with a steady supply, demand and waste generation.

1.2.1 We suggest that

- only emissions and environmental concentrations are quantified for the year 2006

1.2.2 This imply that

- no other years are included in this initial assessment

1.3 Product categories

This dimension concerns what product categories are being included in the study. Figure 10 illustrates this dimension.

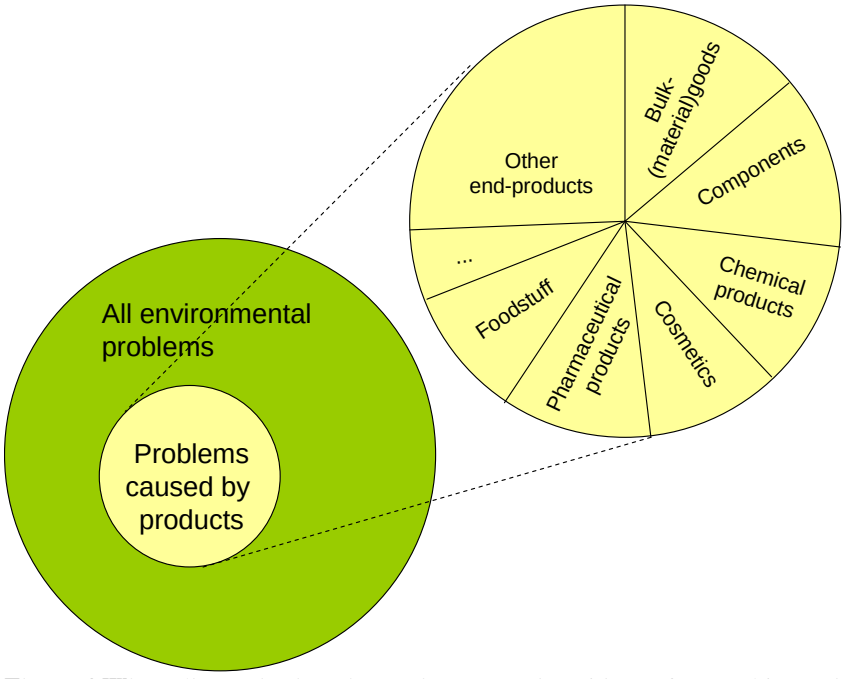

Figure 1 When dimensioning the environmental problem of caused by emissions from products it is necessary to specify what type of products are considered.

The main rationale for including a product category is that products are used in everyday life but still rather unknown from an organic chemicals emissions point of view. This point out typical consumer products such as clothing, furniture, stationary, sports equipment, home appliances, etc. as of specific interest. They and other products like e.g. flooring and some construction materials are represented by the "Other end-products" category in figure 10.

Many products are also used in everyday life but they are excluded based on the rationale that they are already (admittedly with highly varying degree) investigated and managed under various jurisdictions with legal requirements on health or environmental product safety. Cosmetics, pharmaceutical drugs, and foodstuff are hence not included since the interpretation of the scope in Chemitecs is related to the REACH jurisdiction.

Since the system is delimited to emissions of organic chemicals, any product categories that do not contain such chemicals are excluded. This means for example sand and other inorganic ore-based products are excluded. It is acknowledged that such ore-based products are used in very large volumes and since trace amounts of organic substances are present also in these product categories they may contribute significantly to emissions of organic substances. Another very significant material flow is food with its additives and potential emissions of organics from food containers and packaging material, the food itself is not considered "organic substances" (even if it is from a natural science point of view – here the guiding definitions are more related to jurisdictions and policy domains).

In order to make a problem dimensioning a first practical step in the foreseen method for choosing product categories is to take the REACH definition of *articles*[1] as a starting point and match this definition with product categories defined in the CN product category nomenclature [2], in the following referred to as REACH-article categories.

1.3.1 We suggest that

- only emissions from a set of consumer products (REACH-articles) under no specific regulation are included.

1.3.2 This imply that

- emissions from pharmaceuticals, cosmetics, toys, food, and food packaging are excluded despite their significance.

The same approach to match CN can be made for chemical products according to REACH and all other products that are not covered by REACH. Then the next question is – what to compare with what?

In order to answer the question of the dimension of the problem comparisons are necessary. This includes a minimum of two "product use sub-systems" to compare. These systems also need

[1] *"Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorization and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC."* Official Journal of the European Union L396/1, The European Parliament and the council of the European Union.

[2] *"Council Regulation (EEC) No 2658/87 of 23 July 1987 on the tariff and statistical nomenclature and on the Common Customs Tariff"*, Official Journal of the European Union, L 256 , 07/09/1987 P. 0001 – 0675, eur-lex online, http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=CELEX:31987R2658:EN:HTML (accessed 2009-10-05)

to be delimited in ways that makes a comparison reasonable. Furthermore due to the practical (read data availability and acquisition restrictions) the Chemitecs-program is most likely forced to make a comparison of emissions, or predicted environmental concentrations (based on emissions estimates) vs. observed concentrations in some environmental compartments.

Given these initial restrictions there are several meaningful comparisons that can be performed, e.g.:

a. Comparisons between the Chemitecs case-studies (e.g. flooring vs. LCD-screens, regardless of REACH matching)
b. Comparisons between articles according to REACH-article categories and other REACH categories such as chemical products
c. Comparisons between some REACH categories and some non-REACH categories (e.g. REACH-article categories vs. pharmaceuticals)
d. Comparisons between all non-REACH categories and all REACH categories except chemical products for non-household use (many chemical products are only made for professional use)
e. Comparisons between all non-REACH categories and all REACH product categories
f. Comparisons between household product categories and all non-household product categories (i.e. food, cosmetics, pharmaceuticals and some REACH-product categories vs. all the rest).

The consequences in terms of resources pertaining to the different options for comparisons are not fully clear at this point in time. It is however clear that the least demanding is a) and that d) to f) are the most relevant (as judged from the call text of the program and from communications with the programme board). We think that a stepwise approach starting with a) and moving towards f), with checks along the road is advisable.

1.3.3 We suggest that

- a limited number (10-20) of CN-codes (representing REACH-articles) are described in terms of mean-content lists and material transects in order to make comparisons between them and the case-studies possible

1.3.4 This imply that

- the emissions of organic substances from the entire technosphere will be excluded from the initial spring 2010 assessment

1.4 Life-cycle stages/episodes

The handling of system boundaries regarding waste, recycling and packaging will be very important for the outcome.

1.4.1 We suggest that

- only the use stage after installation of products will be covered in the initial assessment
- life-cycle stages (production, use, waste treatment) will be investigated only for case-studies

1.4.2 This imply that

- For most covered articles production is excluded

1.5 Materials

Any materials that contain organic chemicals that can be emitted and that are applied in products are included in the dimensioning study. However, since the sheer number of different materials is so large it is not feasible to describe in detail the exact chemical composition of them all. Assumptions and approximations must be made in terms of average chemical composition for a set of material types. These entities can then tentatively be combined into products that belong to the product categories defined to belong to the Chemitecs-scope.

1.5.1 We suggest that

- only materials for which reasonable mean-content lists can be achieved are covered

1.5.2 This imply that

- many materials cannot be covered.

1.6 Chemicals

The program is by definition delimited to organic (carbon-based) chemicals. There is a gray-zone of what is considered as organic chemicals and organo-metallic substances are within the scope of ChEmiTecs while inorganic carbon-species are not. However, for practical reasons (e.g. lack of physical-chemical data) and time constrains the organo-metallic substances were not considered as case-chemicals and may be studied to a lesser extend than some pure organic compounds.

All organic chemicals that are used in articles can be considered in the program. 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 given the. 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. However, additional organic chemicals with significant emission rates or emission potential will most likely be identified during the course of the program and these will also be considered.

The next step is to further focus on a smaller number of substances, namely those found in the most important materials.

1.6.1 We suggest that

- only emissions of a small set of purely organic substances is calculated (the set may be considerably larger than the number of substances included in the case-studies if it turns out to be feasible to construct mean-content lists)

1.6.2 This imply that

- most organic substances are excluded in this initial assessment

1.7 Use types

Humans are very inventive and quite often use products outside of their intended function. It is however very difficult to account for all such uses why only the types of uses that normally happen to a product, i.e. uses related to the intended function of the product and passive "storage" are included.

Extraordinary use types are excluded in a first approximation: accidents, catastrophic failure of the product, explosions, incineration of products in burning buildings, etc.

Data on unmanaged waste streams are scarce. Therefore littering, burning in open fires, and dumping are emissions that are excluded from the study in a first approximation.

1.7.1 We suggest that

- only emissions from normal intended use and ordinary waste treatment are included. A baseline of passive usage and when deemed that it significantly affects emissions from the product: cleaning/maintenance and uses implying particular emissions are included

1.7.2 This imply that

- emissions from rare or non-intentional use and unmanaged waste streams are not covered. Other uses than cleaning/maintenance and uses implying particular emissions are excluded

1.8 Use environments

Depending on the intended use of a specific product category a match to the actual use environments are made. However, as every specific environment is unique it is not feasible to mimic this vast variability. The model approach is to define a set of typical use environments with different temporal variation of temperature, light and humidity representing the "normal" or intended use environments. Both air and water environments are included. Included here are a set of indoor environments: home, office, car cabin etc.

A set of Swedish outdoors environments covering the location of the bulk of products when used are included.

The exact set of use environment applied in the study is not fully defined at this point in time but delimitations are foreseen. Extreme variations in outdoor use environments such as hurricanes, heat waves, etc. will be excluded. The variation between indoor use environments in industrial production facilities, military situations, hospitals, etc. are not taken into account in the first approximation.

1.8.1 We suggest that

- A very small set of indoor and outdoor environments (approx. 6) are identified in terms of the most important factors (temperature and ventilation) influencing emissions

1.8.2 This imply that

- most environmental variability is omitted and that factors like light and humidity are not varied.

1.9 Emission processes

Emission processes include

- Molecular emission from surface materials in products mainly driven by temperature and concentration gradients between the material in the product and the surrounding use environment.
- Particular emission due to abrasion or similar mechanisms. The particles in turn cause molecular emissions. Based on an increase in surface area of the particulate material

compared to the solid bulk material total molecular emissions will increase from particulate matter.

Other emission processes are at this point not included in the first approximation study such as emissions driven by ultraviolet light, or transfer through direct contact with dust particles or humans (dermal, oral, etc).

1.9.1 We suggest that

- only emissions driven by concentration differences between bulk material and bulk air/water are quantified in this first step. In case of air environments the ventilation is taken into account as a variable boundary layer thickness.

1.9.2 This imply that

- emissions from bulk materials to organisms via direct contact (dermal, oral etc) or emissions mediated by cleaning activities, or partitioning processes are omitted at this stage
- emissions driven by ultraviolet light etc are omitted

1.10 Environmental processes

The study will quantify the emissions as such and the resulting concentrations in different environmental compartments. The concentrations will be quantified by using fugacity models taking into account environmental processes of mass transfer between compartments and biotic and abiotic degradation etc. Further calculation of processes of exposure and toxic effects caused by concentrations is severely hampered by lack of toxicity test data. It is not foreseen as possible to provide verifiable quantitative results of such effects. Therefore the first approximation will calculate emissions. As a second step concentrations in Swedish environmental compartments will be calculated.

1.10.1 We suggest that

- emissions are quantified in a first step
- environmental concentrations are quantified in a second step using fugacity model

1.10.2 This imply that

- (eco)toxicological effects of any kind are excluded in this initial assessment

1.11 Environmental problems

The effects in the environment due to emissions of organic chemicals span over a wide spectrum. In addition to adverse responses such as cancer, allergy, reproduction inhibition, etc. other effects are also caused by these chemicals including eutrophication, ozone layer depletion, etc. However, any further quantification than the emissions themselves and, as a second step, the resulting environmental concentrations are not foreseen to be extensively studied due to the known data gap. One approach is to apply characterisation factors from LCIA models to obtain a first estimation of effects but even this need toxicity data that are still not available.

1.11.1 We suggest that

- only emissions and environmental concentrations are quantified in this first step

1.11.2 This imply that

- no effects of any kind are included in this initial assessment