Emissions from Articles

Synthesis report of the ChEmiTecs Research Program

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Rapport

Emissions from Articles

Synthesis report
of the ChEmiTecs Research Program

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Preface

Organic **Ch**emicals **Emi**tted from **Tec**hnosphere Article**s** (ChEmiTecs) was a research program funded by the Swedish EPA which ran during the years 2008-2013. The goal of the program was to improve the understanding of mechanisms, magnitude and implications of emissions of organic substances from technosphere articles. It was also aimed at supporting the development of Swedish and EU management programs to minimise risks from harmful substances. ChEmiTecs has been the first research program to assess, on the National scale, the magnitude of the problem of emissions of chemicals in materials and articles. The issue was brought forward in the 1990-s as part of discussions between The Swedish EPA and The Swedish Chemicals Agency (KemI), later elaborated in the investigation in SOU 2000:53 (Varor utan faror). Subsequently the research program was launched.

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Summary

Environmental risk posed by emissions of chemicals contained in products is an important issue that has been, so far, investigated to a relatively limited extent. In response, the research program ChEmiTecs was set up specifically to improve the understanding of mechanisms, magnitude of emissions on the national Swedish scale, as well as perception about, and management strategies of emissions of additives and other organic substances from articles to the environment.

Additives are, as the name indicates, added to a material. This is done with a purpose to improve the properties of the product in its intended use. The societal benefit of, e.g., flame retardants is immense as they contribute to reduce the risk of fire. In order to maintain the purpose of the additive, it should stay in the product. The fact that additives are nevertheless released to some extent is therefore rather an unwanted consequence.

In order to understand the mechanisms and magnitude of the emissions, different methods were combined:

A product – material – substance inventory was developed of the flows and stocks of the relevant articles and their material constituents with their content of relevant substances, typically organic functional additives. The inventory was based on national trade statistics and well-informed estimates of life length, areas of the articles, and additive content as inventory elements. The research showed that it is possible to use national trade statistics as a starting point to estimate societal stocks of additives, and a total amount of 3×10^6 tonnes of organic chemical additives was estimated to be stored in plastic materials in articles within the Swedish technosphere. Product categories of particular interest are plastic products such as pipes and hoses, films and boards, and the plastic components of other products such as insulated wires and cables, furniture (sofas), and passenger cars including tires. Chemicals stored in large amounts are typically plasticizers (including the groups phthalates and adipates), organic pigments and flame retardants (for example brominated or phosphorous-based flame retardants).

Computational models were applied for calculating product-group and nation-wide emissions based on the inventory. A simple model selected from literature was used to provide a rough estimate with the widest possible coverage for National scale emissions with manageable data need. An advanced computational model was also developed in the program. This model was calibrated by controlled emission chamber experiments for a small sample of test cases, and was then applied to a limited number of detailed product inventories. Results of these data-intensive calculations in the advanced model were also validated against measured concentrations in the environment. The results were then compared with results of the rough model, to get an idea of the accuracy of the national estimate. The ChEmiTecs assessments indicate national molecular emissions to air of plastics additives from the societal stock of material and products

during their service life to be in the order of 500 tonnes per year. As an approach to getting an idea of the severity of these emissions, a comparison was made with intentionally released biocides. As chemical substances may have very different properties in terms of potential harm to the environment, a direct comparison in terms of mass flow is not very meaningful. Instead, substance emissions were recalculated to ecotoxicity scores with a model developed in the life cycle assessment science domain. The scores obtained indicate lower overall ecotoxicity potential of emissions of additives on the national Swedish scale compared to biocides. The results need to be taken with great precaution as there were significant data gaps. Emissions from waste and waste management were also not included in this calculation.

The mechanisms determining the emissions are complex. But at least the results from the research confirm some basic circumstances:

- Products with a large surface area (e.g. upholstered furniture, pipes and hoses, polymer films, etc.) were identified to favour emissions. Given a certain combination of material and additive, the emissions will be roughly proportional to the area of the object.
- Smaller molecules are more likely to be emitted than big ones. “Small” and “Big” may refer to the molecular weight, but also to the shape of the molecule, so that stretched out molecules with long branches are getting more entangled in the matrix material than compact molecules with short branches, and therefore tend to emit more slowly.
- Higher temperature will typically result in higher emissions, which was exemplified with releases of Tri-phenyl-phosphate (TPP) from flat computer screens.
- The specific affinity of the additive to the matrix material is important, but it is a complex issue, as it depends on properties for both the additive and the matrix.
- An additive’s tendency to transfer to the surrounding medium is typically expressed as a partitioning coefficient. For semi-volatile and low volatility chemicals, to which groups additives often belong, the release rate is more determined by the molecule’s tendency to transfer from the surface to the surrounding medium than the migration rate within the matrix.

To summarize, it appears evident that the combined properties of the material and the molecule as well as the surrounding conditions are crucial for the emissions.

Emissions from articles cannot fully explain the environmental occurrence of the substances in a certain location or Nation, thus other sources such as direct industrial releases and/or atmospheric long-range transport may be equally or more important. However, in the indoor environment, consumer products including building materials are more or less the sole sources of many organic chemicals, and may thus have a significant contribution to overall human exposure. Chemicals of particular interest are plasticizers and flame retardants, e.g. phthalates and organophosphates. Common for these substances are that many of the products they occur in are used in the indoor environment (plastic flooring, furniture).

Accounting for article lifetime and typical release rates as calculated in ChEmiTecs and supported by other work in literature indicates very clearly that more than 90 % and in most cases more than 99 % of the added chemical additives remain in the products at the end-of-life, which means that the major share of the originally added substance of the substances will enter the waste and recycling streams. This is important to consider as they may be eliminated if the products are incinerated, or re-circulated into new materials and products if the material is recycled.

According to the surveys conducted within the program with consumers and producers during the year 2012, emissions from articles are not generally perceived to be of major concern from a health or environmental perspective. Producers were of the opinion that they have the necessary tools to perform risk assessments, and they are reasonably content with the current legislation. Consumers were mostly concerned with potential risks for workers and to the local environment near production plants.

Studies carried out within ChEmiTecs also showed that the Swedish environmental goals are in general terms not important drivers towards voluntary agreements to change chemical contents in consumer articles. Here, stricter requirements are therefore needed to promote change.

The following recommendations were formulated on the basis of the outcome of the research:

- The accessible information about content of additives and other chemicals in articles is quite limited. Supply chains consist of several steps, and companies selling articles on the market are often not aware of the additives content of their products. Article 33 in REACH is in theory a mechanism requiring such companies to know their articles' content. Ideally, this additive content information should be combined with the collection of statistical information on trade. A requirement from authorities and a registry of additive content in articles, analogous to the "Product registry" for chemicals and blends operated by the Chemicals Agency, could potentially be a suitable mechanism to push for such information. This is essentially a pre-requisite for reliable estimates of stocks of chemicals from products in the future.

- Within its Environmental monitoring activities, Swedish EPA carries out regular screenings campaigns of chemicals in the environment. Screening activities of chemical content in products would be a good complement, which would contribute to knowledge on additives and other chemicals content in articles. Similarly, we emphasize the need for new requirements on emission testing of a wider range of chemicals. Providing sufficient data availability, the

ChEmiTecs emission model could be an important tool to assist in such assessments.

- It should be evaluated whether product specific rules could be suitable as a complement to REACH for consumer articles where hazardous chemicals are present and the use is widespread, such as textiles and building products.

- Producers should strive to minimize the content of chemicals with hazardous properties in general and in particular in products made of porous materials and/or of large surface areas aimed for use in the indoor environment.

- Emissions from multilayer products and via migration and abrasion need to be further investigated. More recent research indicates that direct migration to dust can contribute significantly to the levels found in the indoor environment.

- Since the major share of the chemical additives are estimated to remain in articles at the end of their life there is a need for alertness among waste managers and recycling industry to handle this. Information about the content of goods that reach the waste stream could contribute to this.

Sammanfattning

Emissioner från Varor (Organic Chemicals Emitted from Technosphere Articles - ChEmiTecs) var ett forskningsprogram som löpte under åren 2007-2013 och som finansierades av Naturvårdsverket. Målet med programmet var att öka förståelsen av mekanismer, omfattningen och konsekvenserna av utsläpp av organiska ämnen från varor.

I samarbete med myndigheter, tillverkare och nedströmsanvändare identifierades tekniska och sociala aspekter som bidrar till problemet med utsläpp från varor, i syfte att skapa en gemensam förståelse för problemet och dess sammanhang. En urvalsstrategi togs fram i syfte att identifiera problematiska ämnen, varor och användningsmönster. Därefter kvantifierades utsläpp av ett litet urval av ämnen från varor och uppskattades med hjälp av modellbaserad extrapolering för ett stort antal andra ämnen. Betydelsen av dessa utsläpp bedömdes bland annat i förhållande till andra utsläppskällor.

Forskningen visade att det är möjligt att använda den nationella handelsstatistiken som en utgångspunkt för att bedöma mängden av kemiska ämnen som är upplagrade i samhället, och totalt uppskattades den upplagrade mängden av organiska kemiska additiv i plastmaterial i varor i den svenska teknosfären till 3×10^6 ton. Produktkategorier av särskilt intresse är rör och slangar, plastprodukter såsom plastfilm och skivor, isolerade ledningar och kablar, möbler (soffor) samt personbilar inklusive däck. Kemikaliegrupper som är upplagrade i stora mängder är framför allt mjukgörare (inklusive grupper såsom ftalater och adipater), organiska pigment samt flamskyddsmedel (till exempel bromerade och fosforbaserade flamskyddsmedel).

Emissioner av kemikalier från varor bedömdes genom att kombinera olika skattningsmetoder med beräkningsmetoder som kalibrerats med hjälp av kontrollerade experiment samt genom dubbelkontroll där spridningsmodeller anpassades med stöd i empiriska miljödata. De beräkningar som gjorts inom programmet tyder på att den enkla modell som tillämpades för att beräkna emissioner på nationell skala för ett brett antal produktgrupper överskattar utsläppen av plasttillsatser från produkter. Resultat från den mer avancerade beräkningsmodellen som utvecklades inom programmet tyder på att utsläppen från varor i medeltal motsvarar ca 0.2 promille av de additiver som finns upplagrat i varorna. För vissa produktgrupper kan dock utsläppen uppgå till några procent av den upplagrade mängden. Utifrån antagandet att 0.2 promille av de upplagrade kemikalierna emitteras från varor, uppskattades de årliga nationella utsläppen av plasttillsatser i den samlade materialstocken till i storleksordningen 500 ton.

Uppskattningen 500 ton per år enligt ovan måste ses som en grov och relativt osäker skattning, eftersom mekanismerna för ämnens avgång från ett material är komplexa. Det är de kombinerade egenskaperna hos materialet, molekylen och omgivande miljön som är avgörande för utsläppen. Vissa samband kan lyftas fram:

- Produkter tillverkade med en stor ytarea (till exempel stoppade möbler, rör och slangar och bildäck) verkar ge upphov till höga utsläpp.
- Små molekyler emitteras i större grad än stora molekyler. Här hänvisar små och stora molekyler både till molekylvikt men även till molekylstruktur, där avlånga förgrenade molekyler ofta hindras av materialet i matrisen och därmed tenderar att emitteras långsammare.
- Temperatur är en viktig faktor som påverkar utsläppen. Högre temperatur kan leda till högre utsläpp, vilket inom programmet påvisats med försök på utsläpp av trifenylfosfat (TPP) från LCD-skärmar.
- Additivets affinitet till materialmatrisen är en viktig men komplex faktor som påverkar utsläppen, då affiniteten påverkas av egenskaperna hos både additivet och materialet.
- Additiver kategoriseras vanligen som semiflyktiga eller lågflyktiga ämnen. Avgången av dessa ämnen från ett matrismaterials yta verkar avgöras i många fall i högre utsträckning av ämnets benägenhet att gå över till omgivningsmiljön, t ex förångas från ytan, än av migrationshastigheten i matrismaterialet.

Med produktens livslängd i beaktande uppskattades mer än 90 % och i de flesta fall mer än 99 % av de tillsatta kemiska additiven finnas kvar i produkterna i slutet av dess livslängd, vilket innebär att de flesta av additiven kommer in i avfalls- och återvinningsleden. Där kan de elimineras om produkterna förbränns, eller så kan additiven återcirkuleras in i nya material och produkter vid materialåtervinning.

Forskningen inom programmet visar att utsläpp från produkter inte helt kan förklara förekomsten av ämnena i den yttre miljön. Således kan andra källor såsom industriella utsläpp och långväga transport via luft även vara viktiga. När det gäller inomhusmiljön är konsumentprodukter, inklusive byggmaterial mer eller mindre de enda källorna till förekomsten av många organiska ämnen (till exempel ftalater och organofosfater), vilket kan ha betydelse för människors exponering.

Enligt de undersökningar som gjordes inom programmet under år 2012 med avseende på konsumenters och producenters inställning till emissioner från varor är slutsatsen att utsläpp från varor i allmänhet inte uppfattas som ett stort hälso- eller miljöproblem. Producenter var av den uppfattningen att de har de nödvändiga verktygen för att utföra riskbedömningar, och de är ganska nöjda med den nuvarande lagstiftningen, vilken också är den starkaste drivkraften i deras miljöarbete. Konsumenterna var av uppfattningen att riskerna är störst för arbetstagare och den lokala miljön i närheten av produktionsanläggningar. I allmänhet föredrar konsumenter märkning för att kommunicera produktinnehåll.

I syfte att belysa problematiken vad gäller risker för miljön gjordes en jämförelse av möjlig giftpåverkan på vattenmiljö (potentiell ekotoxicitet) mellan plastadditiv och biocider med hjälp av en beräkningsmodell som traditionellt används inom livscykelanalysforskningen. Beräkningarna visar att den totala möjliga giftpåverkan av utsläppta tillsatsämnen från plastprodukter i Sverige är lägre än den är från avsiktligt utsläppta biocider. Dock omfattar denna analys inte alla relevanta effektmått och det var heller inte möjligt att bedöma samtliga plastadditiv på grund av databrist. Utsläpp från avfallsledet finns heller inte med i denna beräkning. I allmänhet är kunskapsluckorna fortfarande stora när det gäller egenskaper och toxicitet av kemiska tillsatser i konsumentprodukter, vilket minskar möjligheten till en gedigen utvärdering och dimensionering av hälso- och miljöpåverkan av kemikalier i varor ur ett riskperspektiv.

Studierna inom ChEmiTecs visade att de svenska miljömålen i sig inte utgör några viktiga drivkrafter för att träffa frivilliga överenskommelser med syfte att ändra kemikalieinnehåll i konsumentvaror.
Studierna indikerade också att marknadstrycket för att få producenter att ändra innehåll är ganska svagt, även om arbete pågår inom vissa branscher. Drivkrafter i dessa fall är typiskt kommande lagstiftning eller förväntad kommande lagstiftning.
Resultat framtagna inom ChEmiTecs-programmet visar även på ett behov av att stärka den produktspecifika lagstiftningen som ett komplement till REACH i syfte att minska riskerna med farliga ämnen för vissa produkter, exempelvis byggprodukter och textilier.

Följande rekommendationer formulerades på grundval av resultatet av forskningen inom programmet:

- Information om additivinnehåll i varor är fortsatt starkt begränsad. I många fall är nedströms varuproducenter också begränsat medvetna om förekomsten av additiver i materialen i sina produkter. Artikel 33 i REACH föreskriver att leverantörer ska kunna förmedla information om ämnen på kandidatlistan över föreskriven halt i sina produkter, vilket indirekt innebär ett krav på att veta det faktiska innehållet i varor. En mekanism för att åstadkomma bättre information om upplagring av additiver i varor i samhällets materialstock, och emissioner av dessa, vore att ha ett register över varors innehåll liknande Kemikalieinspektionens Produktregister för kemikalier och beredningar, kombinerat med dagens statistik över med Industrins varuproduktion och varuimport och –export.

- Som komplement till dagens screeningprogram som mäter upp och övervakar halter av kemikalier i miljön, rekommenderar vi att det via lämpliga marknadskontrollmyndigheter och Naturvårdsverket satsat på ett ”screeningprogram” för kemikalier i varor. En del av en sådan satsning kan också vara att implementera nya krav på utsläppstester, t ex med hjälp av emissionskammare, av ett bredare spektrum av ämnen. Sådana krav kan till exempel kopplas till ovan nämnda produktspecifika lagstiftning, för att driva utveckling mot lägre konsumentexponering från varor.

- Lagstiftare bör utvärdera om produktspecifika regler skulle kunna vara ett lämpligt komplement till REACH för konsumentprodukter där farliga ämnen förekommer och användningen är utbredd, såsom t ex textilier och byggprodukter

- Producenter bör sträva mot att minimera innehållet av ämnen med farliga egenskaper i produkter tillverkade av porösa material eller som har stora ytor, i synnerhet i sådana produkter som är avsedda för användning inomhus.

- Utsläppen från flerskiktsprodukter och via direkt migration till damm samt via slitage behöver utredas ytterligare. Aktuell forskning visar att direkt migration från produkter till damm kan ge ett betydande bidrag till kemikalienivåerna som påvisas i inomhusmiljön.

- Eftersom huvuddelen av tillsatta kemiska additiv bedöms finnas kvar i produkterna i slutet av deras livslängd behöver det finnas beredskap i avfalls- och återvinningsleden att hantera detta. Information om varornas innehåll som även når avfallsledet skulle kunna bidra till denna hantering.

1 Introduction

1.1 Overarching objectives of ChEmiTecs

The research questions raised by the Swedish EPA at the launch of the program were:

- What is the magnitude of the problem related to emissions of organic substances from articles, and how big will it be in the future?
- What combinations of substances, articles and use patterns contribute the most to exposure of humans and the environment in the short and long term?
- In what phase of the article life cycle from use to landfill does the largest release to the environment occur of risk substances?
- What measures are necessary to reduce risk associated with chemicals in articles in a sustainable society? Can articles continue to be used as today or do we have to change their contents or the distribution routes to make the articles fit into the sustainable society?

One of the key issues to address in the ChEmiTecs program was the magnitude of the problem with emissions from articles. In short – are emissions from articles of concern? In collaboration with authorities, producers and downstream users, technical and social aspects contributing to the problem with emissions from products were identified, in order to create a common understanding of the problem and its context. Within the program a selection strategy was developed in order to pinpoint problematic chemicals, articles and use patterns. Next, chemical emissions were quantified for certain chemicals and estimated for a large number of other chemicals by a computational model calibrated by controlled experimental measurements. The importance of these emissions was assessed in relation to emissions from other sources, e.g. industrial facilities and long-range transport.

2 Conceptual framework of the research program

The individual studies conducted under the ChEmiTecs research program all deal with chemicals in articles, their emissions and implications of such emissions. An initial structure, which included definitions of terms and project boundaries, was formulated to clarify the key concepts. This overview of the system studied within the program comprises e.g. the key concepts Product, Chemical, Use and Emission. The main area where ChEmiTecs is concerned is within the technosphere, but the boundaries between the technosphere and the natural system are crossed, since that is where the emissions end up, and the natural system is also where our main endpoints lie (i.e. humans and wildlife and potential effects on these). A brief introduction to these concepts and their definitions within the program is presented in the following, and they are elaborated and complemented further by Tivander et al. (2010).

2.1 Chemical

A *chemical* is defined based on its elemental composition and structure of molecules. Within the REACH legislation (EC, 2006) a substance is defined as "a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition". The chemical substance concerns only the physical structure and properties of elements and molecules. Each chemical has *Chemical properties*, e.g. molecular weight, vapour pressure, melting point, and degradation half-lives in biotic or abiotic matrices. A specific property is the intended *function* of the chemical in a material, e.g. flame retardant, UV-stabilizer, dye, etc. This is of particular interest since many data about the existence of chemicals in products are only documented in terms of chemical function (what the chemical does) and not of chemical composition (what the chemical is).

2.2 Product and article

The main source of emissions targeted in the research program is the *product*. It is defined as "any physical matter that is produced or designed for a use purpose; mostly, but not necessarily, products are traded on a market". This definition is close to the terminology of economics where a tangible (physical) product is "a good" (Swedish: "vara"). A product is the result of a technical (anthropogenic) production process, e.g. assembling components, processing of a material, preparations or reactions of substances. The product is a generic in the sense that it does not exclude any specific types of products. For comparison, the related term *article* is defined by the European Commission (EC, 2006) as "an object which during production is given a special shape, surface or design which determines its function to a greater degree than does its chemical composition". This definition primarily serves to distinguish chemical substances and mixtures from other products which makes the article concept a subset of the product concept. While the conceptual framework is valid for any type of product, the scope of the ChEmiTecs program is limited to a sub-selection of articles. Additional relevant terms that are associated with the product concept are *product category*, *component*, and *material* (**Fel! Hittar inte referenskälla.**). Together, they make up the analytical aggregation levels of how and where chemicals are contained in products and accumulated in society (i.e. the technosphere). This is crucial information needed to define, characterise and quantify emissions of chemicals from articles. In the current report, we focus on the *article* when emissions are assessed.

2.3 Use and product lifetime

The *use* concept encompasses all episodes of how and where products are handled, actively or passively. A clear distinction is made from the concept of product *function* which is an idealized description of the intended use and not necessarily what actually happens to a product. The use of a product is a combination of product (*what* is used) use type (*how* the product is used), use environment (*where* the product is used and hence where emissions occur), and use time (for *how long* the product is used). The product *lifetime* is the total time-span from when a product is created until it enters the waste stream. The lifetime of a given product can be divided into episodes of uses where each use occurs over a time span called use-time. Adding all use-times of a product equals the product's lifetime.

For comparison, the REACH legislation defines use of a chemical substance as: "any processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, production of an article or any other utilisation" (EC 2006).

Within ChEmiTecs, the product life-time is considered as the time between it enters the market until it is classified as waste and thus enters waste treatment stream. For example, the lifetime of building products are considered to be from the entrance in a building market until demolition. Thus, demolition processes are considered part of the waste stage.

2.4 Emission

The absolute central concept of the ChemiTecs Concept Model is the *emission* i.e. the flow of a substance from a source in the technosphere to a receiving compartment in the nature system. An emission thereby implies the loss of human (technological) control of the substance as it becomes subject to the course of nature. The emission concept is well established in environmental discourse, however specific related concepts need definitions such as *emission driver* which include environmental aspects including temperature, light, ventilation, humidity, etc., which may trigger or influence emission and also the type of use such as internal heating when using the product or whether abrasion occurs or not. The *emission pathway* is also relevant and includes phenomena such as diffusion, migration, volatilisation, and abrasion.

Within ChEmiTecs, an *emission* is regarded as a molecular release of a parent compound, i.e. the transport of the additive molecule out of its carrying material into the surrounding environment, which is normally air or water, but could also be other materials or matrices in direct contact with the material, such as skin, household dust or soil solids. Transformation products were not considered in this analysis. Abraded particles are viewed as part of the original article, or rather, as transport vehicles with the special characteristic that abrasion may speed up and enhance molecular emission by increasing the surface area available for release (Figure 0-1).

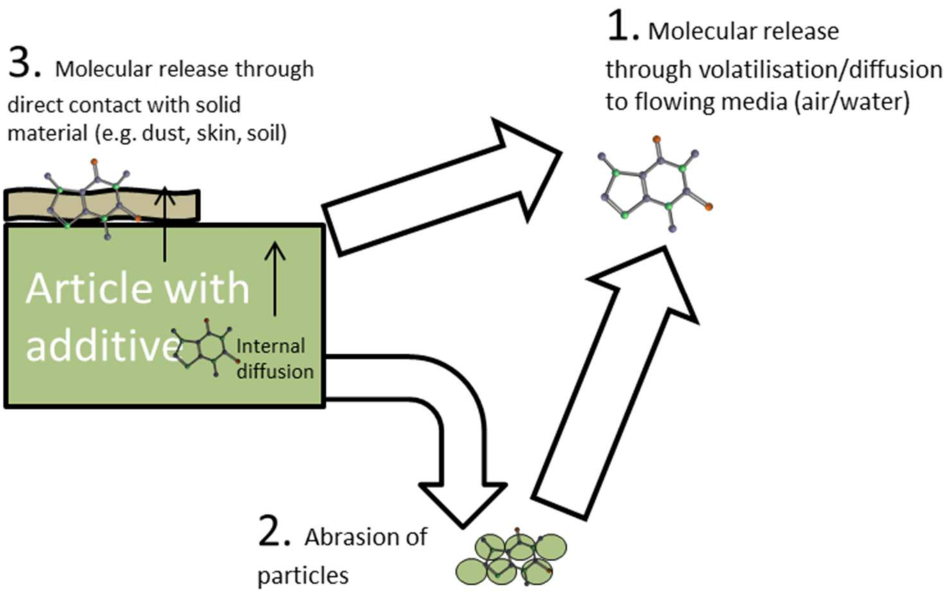


Figure 0-1. Different pathways of emission from an article. Within ChEmiTecs, emission is regarded as the molecular release of an additive into an environmental matrix. This may include molecular release from the article, or abraded particles thereof, through volatilisation or diffusion (1). It also includes molecular release from the article (or its abraded particles) to adhering solid matrices, e.g. dust, human skin or soil solids through direct migration (3). Abrasion is viewed as a transport process which may enhance molecular emissions but is not viewed as an emission in itself. Internal diffusion is the process within the article whereby additives are passively transported to the surface from where it may be released to the surrounding environment.

3 Estimating chemical stocks

3.1 Summary and recommendations

A key to understanding and being able to quantify emissions from consumer articles is to ensure a good estimation of the accumulated stocks of chemicals that are present in technosphere articles. Therefore, a major part of the ChEmiTecs research program was devoted to the development and application of calculation methods to estimate such stocks on a national scale. This chapter demonstrates that in principle, it is possible to use national trade statistics as a proxy. The total amount of organic chemicals stored in consumer articles was estimated to **3×10^{6} tonnes** of chemical additives in plastic articles, and **3.1×10^{5} tonnes** of additives in 16 different product categories related to the selected case study objects presented in Table 0.3. Product categories of particular interest are pipes and hoses, plastic products such as films and boards, insulated wires and cables, furniture (sofas) and passenger cars including tires. Chemicals stored in large amounts are typically plasticizers (phthalates and adipates), organic pigments and flame retardants, but also substances such as melamine, rapeseed oil and stearic acid.

Regarding *material stocks*, there is currently enough information available to estimate the total accumulated stocks, although there is no way to "verify" the calculations since it is practically impossible to weigh all the materials in all products stocked up in the society. It also became evident, that the *material surface* is a crucial parameter for estimating emissions. The general lack of information of chemical content presents a significant obstacle to obtain reliable estimates of *chemical stocks*. Measuring chemical composition of materials is a time-consuming and expensive task and is simply not feasible on an economy-wide scale.

We recommend that the collection of statistical information on trade is complemented by average composition lists (down to CAS-level) for each material, agreed upon by the relevant business sectors. This is essentially a pre-requisite for reliable estimates of stocks of chemicals from products in the future. This recommendation is in line with the joint global initiative "The Chemicals in Products Programme" which was launched in 2015 by WHO/UNEP/SAICM aiming to promote information sharing on chemicals in articles (UNEP, 2015).

3.2 Linking trade statistics to chemical stocks

The basis for the estimating chemical stocks was the national trade statistics as collected and processed by Statistics Sweden (SCB). By using the existing Combined Nomenclature (CN) system and data from the International Trade and the Industrial Production of Goods databases together with expected product lifetime, Sörme et al. (2013) illustrated a method to estimate the accumulated stocks of particular products on an aggregated level (CN4) in tonnes or based on surface area (m^2). Through additional calculations of material contents, the proposed method was further modified, according to the scheme outlined in Figure 0-2. Typical material composition lists were prepared (Figure 0-3). To allow for later emission estimates, a thickness interval and a density was estimated for each identified material selected from a total of ~100 CN4 categories, each of which contains a large number of subcategories.

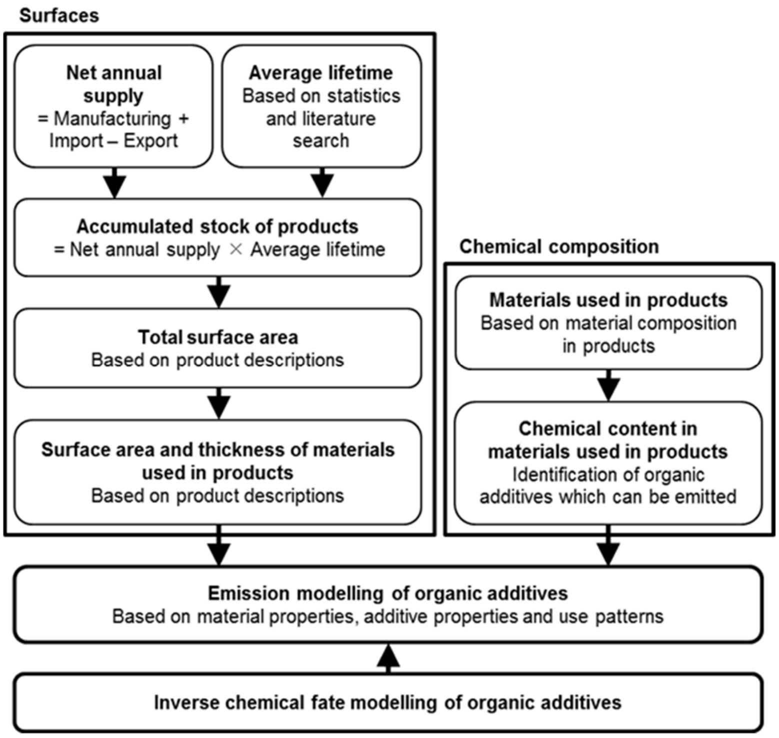


Figure 0-2. Process for estimating emissions of organic chemicals in articles on the national scale. From Molander et al. (2013).

Product	Application	Material
Spring mattress with wooden frame	Outer fabric	Cotton
Spring mattress without wooden frame	Outer fabric	Cotton
Foam mattress	Outer fabric	Cotton
Sofas	Outer fabric	Cotton
Cotton jackets	Outer fabric	Cotton
Cotton jackets	Inner fabric (no lining)	Cotton
Rain jacket (regular and type gore tex)	Inner fabric (no lining)	Galon (Cotton nylon)
Rain jacket (regular and type gore tex)	Outer fabric	Galon (PU/PVC)
Spring mattress with wooden frame	Inner upholstery	Latex
Spring mattress without wooden frame	Inner upholstery	Latex
Foam mattress	Inner upholstery	Latex
Sofas	Inner upholstery	Latex
Rain jacket (regular and type gore tex)	Outer fabric	PA
Rain jacket (regular and type gore tex)	Inner fabric (no lining)	PA
Wool jackets	Lining	PA
Synthetic jackets	Outer fabric	PA
Synthetic jackets	Lining	PA
Spring mattress with wooden frame	Outer fabric	PES
Spring mattress without wooden frame	Outer fabric	PES
Foam mattress	Outer fabric	PES
Sofas	Outer fabric	PES
Office chairs	Outer fabric	PES
Rain jacket (regular and type gore tex)	Outer fabric	PES
Rain jacket (regular and type gore tex)	Lining	PES
Wool jackets	Lining	PES
Synthetic jackets	Outer fabric	PES
Synthetic jackets	Lining	PES
Automotive interior	Floor lining	PES
Automotive interior	Roof lining	PES
Automotive interior	Outer fabric seat	PES
Spring mattress with wooden frame	Outer upholstery	PES (vadd)
Spring mattress without wooden frame	Outer upholstery	PES (vadd)
Foam mattress	Outer upholstery	PES (vadd)
Sofas	Outer upholstery	PES (vadd)
Automotive interior	Upholstery seat	Polyether (PUR flame retarded)
Spring mattress with wooden frame	Inner upholstery	Polyether (PUR)
Spring mattress without wooden frame	Inner upholstery	Polyether (PUR)
Foam mattress	Inner upholstery	Polyether (PUR)
Sofas	Inner upholstery	Polyether (PUR)
Office chairs	Upholstery	Polyether (PUR)
Office chairs	Outer fabric	Wool
Automotive interior	Floor lining	Wool
Automotive interior	Roof lining	Wool
Automotive interior	Outer fabric seat	Wool
Wool jackets	Outer fabric	Wool mix

Figure 0-3. Example of material composition list for different product categories. From Molander et al. (2013)

Plastic material was identified as a material type of special interest, since it is incorporated in a large number of different products, and therefore, special focus was put on this material category. Application of the approach illustrated above generated estimated accumulative plastic stocks of **43 000 000 tonnes** in the Swedish society (Rydberg et al., 2012).

One major weakness of the data collected at Statistics Sweden is that it does not contain any information on the chemical composition of the materials and products declared. Information on use of chemicals is collected by the Swedish Chemicals Agency, but this applies only to chemical substances and mixtures, which may be used in industrial processes as well as in product applications. Considering that many of our commonly used everyday consumer products are imported from other countries, additional information linked to the target articles is required. To tackle this, ChEmiTecs researchers developed so-called "average chemical composition lists" (Figure 0-4), which were based on information from industry, from product declaration protocols, information from Swerea and from Häggström (2000), Lacasse and Baumann (2004) and Zweifel et al. (2009).

	A	B	C	E	F	G	H
8	**Functional chemicals**		**CAS RN**		**Concentration range [r**	**Refere**	**Anm.**
9	**Reactive dyes**	several	several		500-30000	I	0,05-3%
10		several	several		500-80000	I	0,05-8%
11	**Azoic (naphtol) (excl banned arylamines)**	several	several		500-30000	I	0,05-3%
12		several	several		500-80000	I	0,05-8%
13	**VAT**	several	several		500-30000	I	0,05-3%
14		several	several		500-80000	I	0,05-8%
15	**Sulphur**	several	several		500-30000	I	0,05-3%
16		several	several		500-80000	I	0,05-8%
17	**Direct dyes (excl carcenogenic, banned ary**	several	several		500-30000	I	0,05-3%
18		several	several		500-80000	I	0,05-8%
19	**Pigment (excl. Banned arylamines)**	several	several		40000-240000	II	
20	***Arylamines from cleavable azo dyestuffs***	Restricted 20 mg/kg	several				
21		2,4-xylidine	95-68-1				
22		2,6-xylidine	87-62-7				
23		2-Naphthylamine	91-59-8				
24		3,3-Dichlorobenzidine	91-94-1				
25		4,4"-bi-o-toluidine	119-93-7				
26		4,4-Methylene-bis[2-chloro-aniline]	101-14-4				
27		4,4-Methylenedianiline (MDA)	101-77-9				
28		4,4-Methylenedi-o-toluidine	838-88-0				
29		4,4"-oxydianiline	101-80-4				
30		4,4"-thiodianiline	139-65-1				
31		4-Aminoazobenzene	60-09-3				
32		4-chloroaniline	106-47-8		20-21	VII	
33		4-Chloro-o-toluidine	95-69-2				
34		4-methoxy-m-phenylenediamine	615-05-4				
35		4-methyl-m-phenylenediamine	95-80-7				
36		5-Nitro-o-toluidine	99-55-8				
37		Benzidine	92-87-5				
38		Biphenyl-4-ylamine	92-67-1				
39		o-Aminoazotoluene	97-56-3				
40		o-Anisidine	90-04-0				
41		o-Dianisidine	119-90-4				
42		o-Toluidine	95-53-4				
43		p-Cresidine	120-71-8				
44	***Carcinogenic dyestuffs***	Restricted 20 mg/kg					
45		C.I. Direct Black 38	1937-37-7				
46		C.I. Direct Blue 6	2602-46-2				
47		C.I. Direct Brown 95	16071-86-6				
48		C.I. Direct Red 28	573-58-0				
49	***Other restricted dyestuffs***	Restricted	several				
50		Navy Blue	118685-33-9				
51	***Restricted Pigment***	Restricted	several				
52		4,4""-bis(dimethylamino)benzophenone	90-94-8				

Textile material overview | Cotton | Polyester (PET) | Polyamid (PA) | PU | Galon PVC | Latex | Wool | Blad8

Figure 0-4. Example of average chemical composition list for the textile component cotton.

By combining the average composition lists with the estimated volumes (area×thickness) of the materials/articles in question, using correction factors to account for the fact that not all plastic articles contain all types of additives (**Fel! Hittar inte referenskälla.**), it was possible to achieve an estimate of accumulated chemical amounts in a large number of technosphere articles. The estimates were conducted according to an iterative process and for plastics, this generated a final estimated tonnage of **3×10^6 tonnes** of chemical additives in plastic articles in Sweden (Rydberg et al., 2015; Rydberg et al., 2012). The majority of these additives were estimated to be stored in pipes and hoses (CN3917), in plastic films and boards (CN3920), in insulated wires and cables (CN8544) and in furniture (CN9403), and are dominated by plasticizers, organic pigments and bromine-based flame retardants (**Fel! Hittar inte referenskälla.**). Approximately half of this amount is attributed to phthalate esters, brominated flame retardants and stabilisers.

Table 0.1. Correction factors used to account for the fact that not all plastic products contain all types of additives

Function	Correction factor

Pigment	0.5
Flame retardant	0.1
Antioxidant	1
UV Stabiliser	0.1
Whitening agent	0.1
Stabiliser, bio	1
Stabiliser	1
Plasticiser	0.5
Stabiliser, secondary	1
Antistat	0.1
Lubricant	0.1
Slip Additive	0.1
Antifogging Additive	0.1
Antioxidant,secondary	1
Filler	0.1

Table 0.2. Estimated annual net inflow and accumulated stocks of chemical additives in plastic articles.

Additive	Net inflow (1000 tonnes/year)	Stock (1000 tonnes)
Antioxidants	**8.2**	**140**
Flame retardants	**36**	**450**
Br-based	*31*	*350*
P-based	*4.0*	*80*
Other FR	*1.0*	*20*
Organic pigments	**38**	**480**
Plasticisers	**66**	**1100**
Phthalate esters	*33*	*550*
Others	*33*	*550*
Stabilisers	**25**	**370**
UV stabilisers	**1.2**	**18**
Other organic additives	**<10**	**<200**
Total	**180**	**2700**

3.3 Calculation of stock and measurements of chemical contents in selected case study objects

To enable more detailed analysis and experimental studies of articles representing a wider range of chemicals, materials and articles on the market, representative case study objects were systematically selected (Andersson et al., 2009; Andersson and Rännar, 2009a; Andersson and Rännar, 2009b; Rännar and Andersson, 2010; Rännar et al., 2008). The case studies formed the basis for the development of a sophisticated emission calculation model and they were also used as examples to illustrate the importance of emissions from articles relative to other source categories. By combining a criteria-based iterative selection process for relevant materials (using criteria such as volume, tonnage, assumed chemical content, availability and different use aspects) with a similar approach for chemicals (using criteria such as physical-chemical properties, long-range transport potential as well as persistence, bioccaumulation and toxicity) (see Figure 0-5), six case-study objects were selected (Table 0.3) representing a product category and a key chemical of interest. These case study objects were subject to further detailed analysis regarding material composition and chemical content.

The calculation method described by Sörme et al. (2013) was exemplified by application to LCD screens, car tyres and impregnated jackets (Brolinson and Carlsson, 2010). It was also applied to PVC flooring materials (including PVC-lined wallpaper), yielding a total surface area of 3×10^8 m^2 in the year 2006 (Sörme et al., 2013). In total 16 CN4 categories were identified to belong to or be closely related to the selected case study objects in Table 0.3. Applying the calculation approach to these 16 categories, resulted in estimated chemical stocks of **3.1×10^5 tonnes** of chemical additives (28 **-** 1.0×10^5 for different product categories) (Rydberg et al., 2015; Rydberg et al., 2012), where sofas, passenger cars and tires on vehicles were calculated to store the majority of the substances (Figure 0-6a) and with melamine and tris(1-chloro-2-propyl)phosphate (TCPP) as the two dominant substances (Figure 0-6b). This information was later used as input to the ChEmiTecs emission model described in 4.3.2.

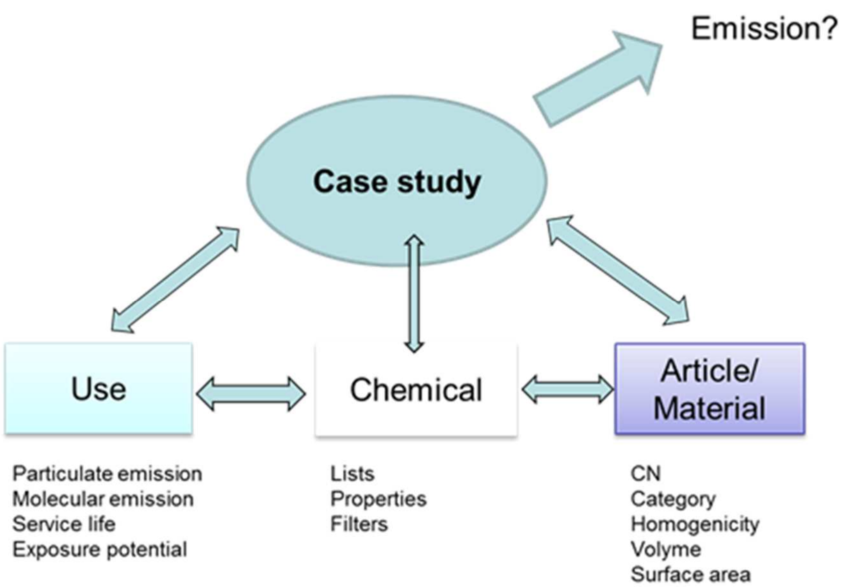


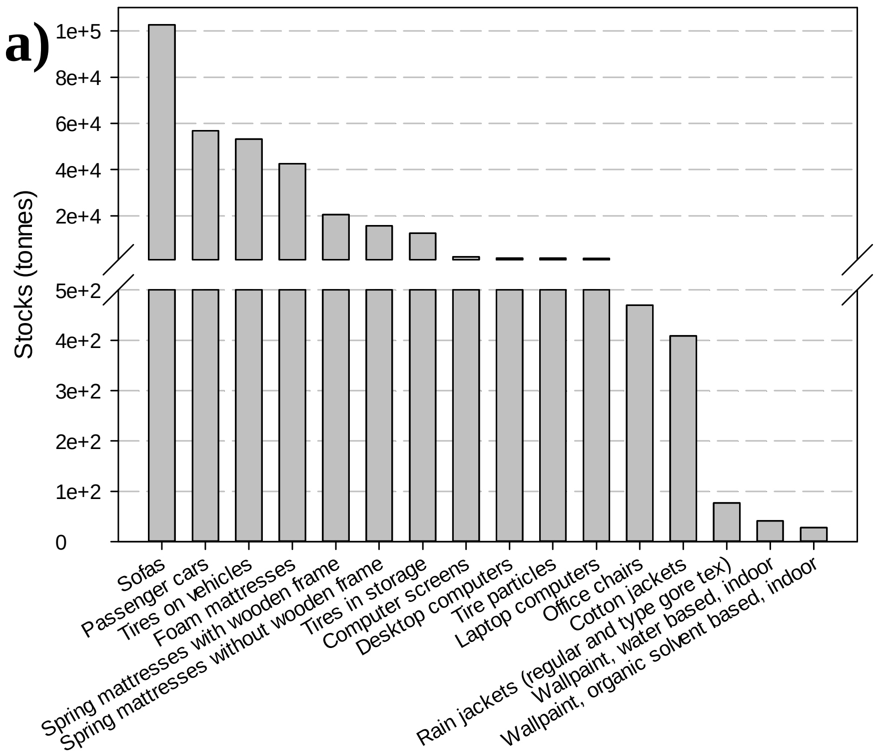
Figure 0-5. Schematic illustration of the different parts of the case study selection process.

Table 0.3. Selected article/chemical combination for use as case-study objects.

Product	CN category (level 4)	Key chemical of interest	CAS
1) PVC floors	3918	Diisononylphthalate (DINP)	68515-48-0, 28553-12-0
2) LCD-screens	8528	Triphenylphosphate (TPP)	115-86-6

3)	**Concrete for underwater applications**	6810	Tributylphosphate (TBP)	126-73-8
4)	**Car tyres**	4011	Mercaptobenzothiazole (MBT)	149-30-4
5)	**Functional jackets**	6101	8:2 fluorotelomeralcohol (8:2 FTOH)	678-39-7
6)	**Indoor paints**	3208	Diuron	330-54-1

As a complement to the detailed desktop studies on chemical stocks in case study objects, a limited number of empirical measurements of chemical contents in products were also performed where chemical contents of and emissions from case study objects were studied. In the work by Holmgren (2013), the contents of polymers and organophosphates (including TPP) in flat panel displays as well as the contents of DINP in PVC flooring material were measured. The average content of TPP in flat panel displays was about 25% (w/w), but seemed to be lower in the more recently produced panels (Holmgren et al., 2013b). The measured content of DINP in floors (13±1.1 % (w/w)) agreed well with the reported concentrations in the floor companies product declarations (16±3.5 % (w/w)) (Cousins et al., 2014). The measurements were used in the further development of the Chemitecs emission model (see 4.3.2).



b)

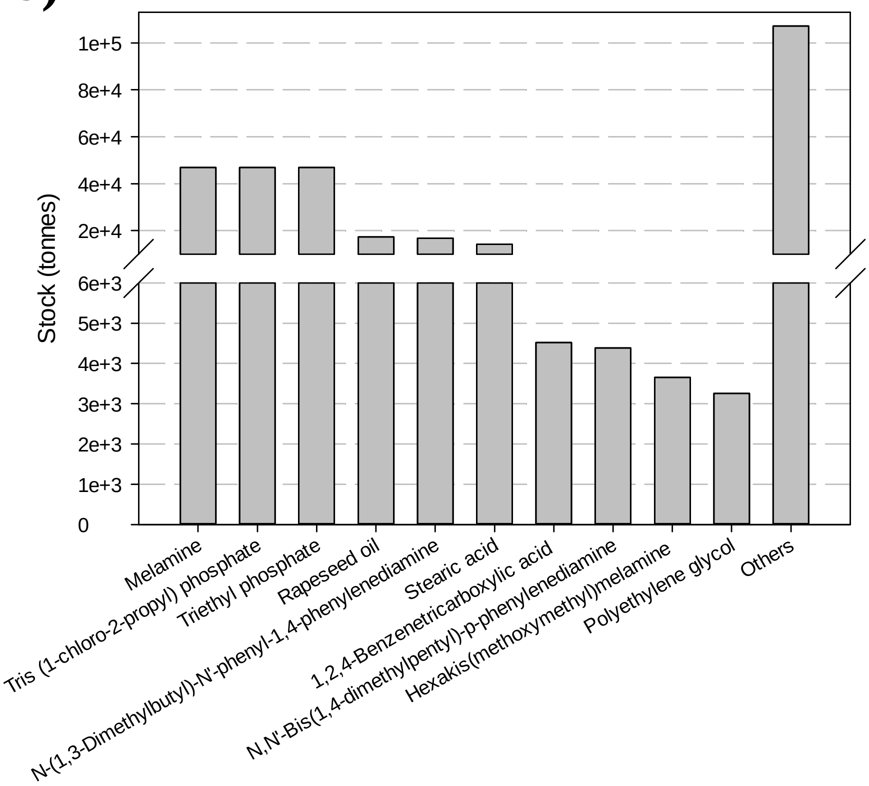


Figure 0-6. Estimated tonnage of chemical additives in 16 selected product categories in the order of a) dominant product categories and b) dominant chemical substances.

4 Estimating emissions

4.1 Summary and recommendations

Emissions of chemicals from consumer articles are best assessed by combining different estimation methods and should be cross-checked through fitting fate models against empirical monitoring data. The ChEmiTecs assessments indicate that the OECD model overestimates emissions of plastic additives from products, approximately by a factor of 100, and final estimates indicate annual national emissions of **500 tonnes**. There is no clear linear relationship between the accumulated chemical stock and the emissions of chemicals. Instead, it appears evident that the combined properties of the material and the molecule are crucial for the emissions. Somewhat simplified, it can be stated that products made of porous materials and/or products with a large surface area (e.g. upholstered furniture and pipes and hoses) favour emissions of molecules with weak binding properties to the matrix in question, which is associated with e.g. low molecular size and high volatility (i.e. low K_{OA}). The modelling and measurement activities within ChEmiTecs further indicated that higher temperature can result in higher emissions, which was exemplified with releases of TPP from LCD screens. Chemicals of particular interest are again plasticizers and flame retardants, but also melamine. Common for these substances are that many of the products they occur in are used in the indoor environment, thus indoor air is likely to be the main recipient.

Emission chamber studies are important complements to study emissions that have been highlighted as potentially problematic, and should ideally be used already in the product development stage. It may be worth considering making emission chamber measurements mandatory for marketing of products containing chemicals with certain properties under REACH. Emission chamber studies are also useful tools to verify or improve model estimates.

Accounting for product lifetime revealed that more than 99 **%** of the added chemical additives remain in the products at the end-of-life, which means that the majority of the substances will enter the waste and recycling streams where they may be eliminated or re-cycled into new materials and products.

We recommend that the collection of statistical information on trade should also be complemented by typical surface areas for each material, agreed upon by the relevant business sectors, i.e. when reporting statistics for e.g. “flat-panel display” it should also be reported what the typical/average surface area for a “flat-panel display” is. We also emphasize the need for new requirements on emission testing of a wider range of chemicals, the results of which should accompany the delivery of material data. This is essentially a pre-requisite for reliable estimates of emissions of chemicals from products in the future. Providing sufficient data availability, the ChEmiTecs emission model could be an important tool to assist in such assessments due to its flexibility and generic design. Additional development required to achieve this includes the expansion to deal with multilayer materials and physical abrasion processes.

4.2 Two approaches to estimate emissions: bottom-up vs top-down

To estimate emissions from articles from accumulated chemical stocks requires many different considerations which may be quite complicated. First, release mechanisms of chemicals from articles depend on a combination of properties of the material and the chemical as well as the conditions in the surrounding environment (e.g. humidity, temperature, flow of receiving media etc.). Second, chemicals which are incorporated in multilayer products (e.g. in PUF material covered by one or two layers of textile), have to cross several boundary layers before they reach the material surface. And third, the amount of scientific literature on different emission mechanisms (volatilisation, abrasion, migration to dust) is limited. In addition, estimating emissions on large geographical scales often requires numerous simplifications and assumptions. As pointed out in Cousins (2013), using combined approaches to determine the magnitude of emissions is advantageous, since all existing emission estimation methods are inherently uncertain. Most bottom-up approaches (i.e. from source to emission) suffer from the inherent weakness that they do not provide any control point, i.e. there is no obvious way to verify the emission estimates, even if specific predicted emission rates may be verified (or derived) by measurements, as shown in chapter 4.3.2. Top-down approaches generally involve the use of a chemical fate model, where an observed environmental concentration is used as a starting point and the model, parameterized to the environment of interest, is used inversely to elucidate the level of emission required to generate the observed concentrations. The limitation is that inverse modelling does not provide any information about the crucial sources (e.g. specific consumer products). By combining bottom-up methods with top-down approaches or inverse chemical fate modelling (Figure 0-7) it is possible to evaluate the overall level of emissions and in the ideal case (with sufficient source-specific data) also identify the most important sources. The top-down approach also provides a possibility to highlight additional emission sources if current emission estimates are considered to be of high certainty and there is a lack of agreement between the different types of estimates.

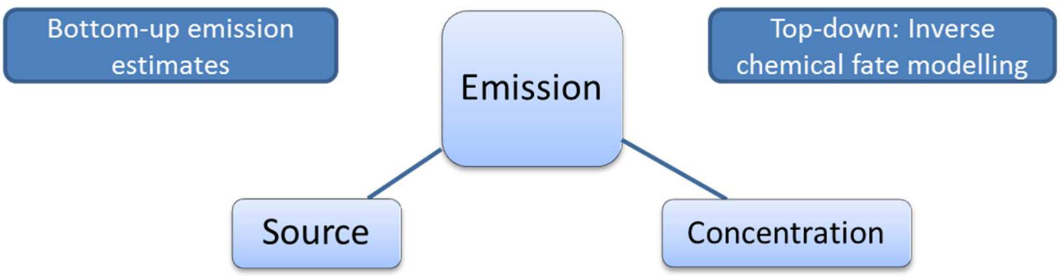


Figure 0-7. Illustration of how bottom-up and top-down approaches complement each other in estimating chemical emissions.

Altogether, the poor knowledge base within the area of emissions from products encouraged the ChEmiTecs scientists to try out different approaches to deal with the issue. As was the case for estimating chemical stocks, the work was performed using theoretical as well as experimental approaches, and represented bottom-up as well as top-down approaches. The results obtained from these parallel tracks are presented in the following sections.

4.3 Bottom-up approaches to estimate emissions

In order to address the two goals of completeness and accuracy in estimating the emissions, two parallel approaches were undertaken to estimate economy-wide emission of chemicals from consumer products, using trade statistics from the Combined Nomenclature (CN) combined with the previously developed composition lists to generate input data:

1. The OECD emission model approach, with low data requirements (see chapter 4.3.1), which was applied to essentially all plastic products on the Swedish market
2. The ChEmiTecs Emission Model approach, the development of which was based on empirical measurements and material diffusion theory. With its higher level of sophistication, data requirements were higher. This model was applied to the 16 product categories (Figure 0-6) related to the case study objects for which sufficient input data was available.

4.3.1 The OECD emission model

The starting point for this approach was the chemical contents in products as described in section 3.1. To achieve a first overview and a rough estimate of the potential amounts of chemicals that may be released from articles in use, we applied a method recommended by OECD (2009), which is based on Fick's second Law of diffusion and utilises the area, the chemical content and the density of the material as well as the molar weight of the chemical as given in Westerdahl et al. (2010). Using this model, the emission of plastic additives from the polymer surface as a result of passive diffusion in the polymer is obtained. In the model, it is assumed that the additives are uniformly distributed within the polymer and that the additives are not chemically bound to the polymer. It is also assumed that the polymer is not subject to physical or biological degradation (OECD, 2009). In calculating the annual emissions for the accumulated stock, we assumed a steady state situation, i.e., that the stock does not change over time, according to equation 3,

$$\frac{Emission}{Year} = \frac{N_{add}(t = averagelifetime)}{Averagelifetime} \qquad \text{(Eq. 3)}$$

where N_{add} is the emitted amount of an additive (kg) at time t, which is governed by the chemical content, the surface area and the molecular diffusivity (which in turn depends on the molecular weight). This calculation method generated estimated emissions of chemical additives from plastics of about **50000 tonnes** per year (Rydberg et al., 2015; Rydberg et al., 2012). Approximately 70% of these emissions were estimated to come from the ten most dominant product categories displayed in Figure 0-8, with largest dominance of plastic films and boards and insulated cables. Table 0.4 displays the typical additive categories, responsible for these emissions where plasticizers are estimated to account for about 50 % of the total estimated emissions from plastics. Stabilisers, organic pigments and flame retardants are estimated to account for 10-15 % each.

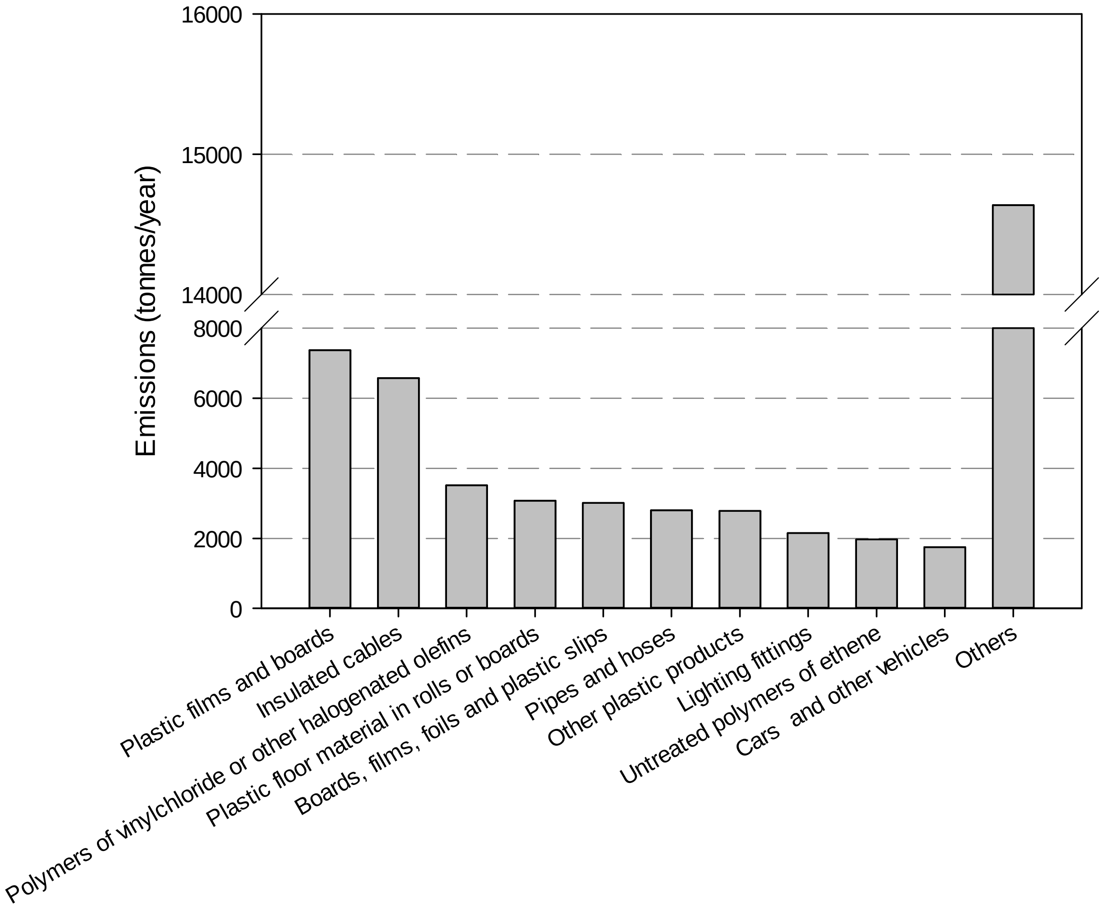


Figure 0-8. Estimated emissions of chemical additives from 10 dominant plastic product categories, using the OECD emission model (Rydberg et al., 2015; Rydberg et al., 2012; Westerdahl et al., 2010).

Table 0.4. Estimated total emissions of chemical additives from plastic products in use, using the OECD emission model (Rydberg et al., 2015; Rydberg et al., 2012; Westerdahl et al., 2010)

Additive	Emission (1000 tonnes/year)
Antioxidants	0.66
Flame retardants	5.6

Br-based	*3.7*
P-based	*1.6*
Other FR	*0.3*
Organic pigments	**6.9**
Plasticisers	**24**
Phthalate esters	*13*
Others	*11*
Stabilisers	**8**
UV stabilisers	**0.36**
Other organic additives	**<1**
Total	**47**

In Figure 0-9, the relationship between estimated emissions and estimated stocks for individual chemicals are plotted. Although higher stock generally results in higher emissions, there is no clear linear relationship between the two. A high accumulated chemical stock can still generate low emissions if the chemical diffusivity is low enough. In contrast, low chemical stocks rarely favour high chemical emissions according to this estimation method.

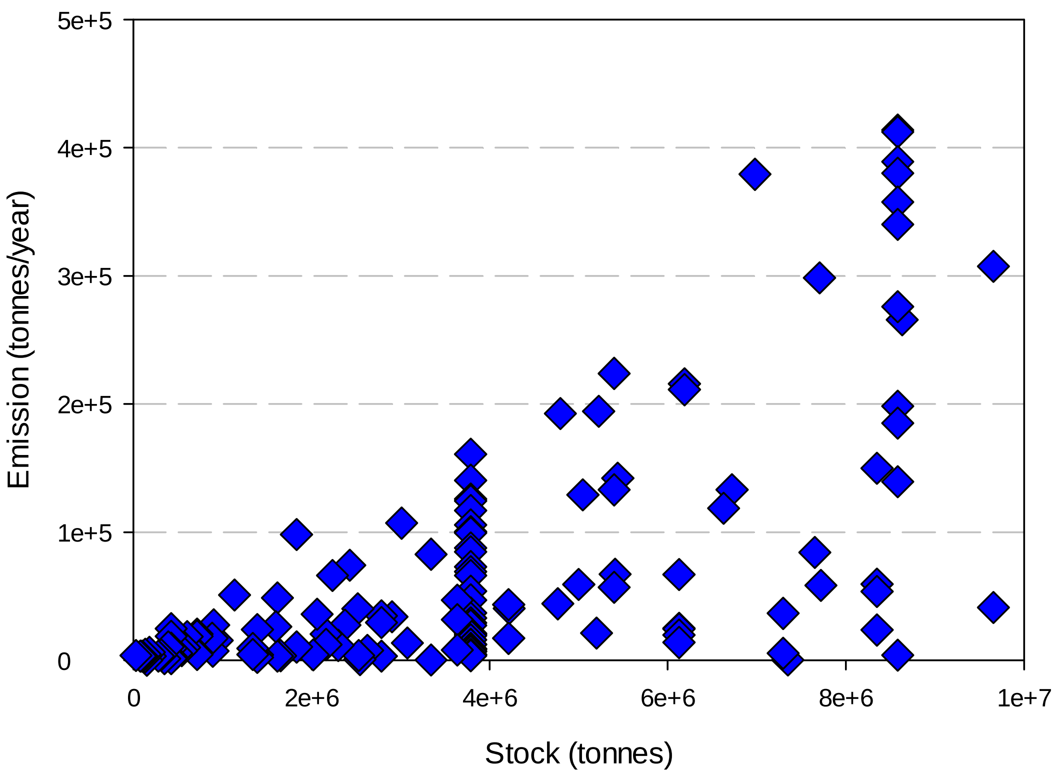


Figure 0-9. Relationship between estimated emissions to air and estimated stocks of chemical additives in plastic products in use.

4.3.2 ChEmiTecs emission model

Although the OECD emission model provides a rough estimate of potential emissions, it became evident that it suffers from substantial uncertainties:

a) It does not consider material and environmental properties, which may affect the diffusion process, and thus the size of emissions
b) It uses a simplified estimation method of diffusivity, only based on molecular weight, although diffusion also depends on the properties of the matrix
c) It assumes a steady state situation which is rarely the case for consumer products
d) It does not respect the fundamental concept of conservation of mass (more than 100% may be emitted)

For this reason, a second approach was undertaken, whereby a generic, mechanistic emission model (the ChEmiTecs model) was developed aimed to enable more specific, verifiable emission estimates of organic chemicals from a large selection of products of varying types. The ChEmiTecs model was designed to predict molecular emissions and considers three key processes: diffusion in the material, equilibrium partitioning at the boundary layer and convection mass transfer in the receiving medium (Figure 0-10). In principle, the model can estimate molecular emissions of any organic chemical from any type of single-layer flat material to any flowing receiving media (i.e. water, air). In its current form the model cannot deal with emissions from multilayer products, nor does it include algorithms to estimate the losses by abrasion. The ChEmiTecs model can, however, be applied to abrasion derived particles, providing that the mass transfer coefficient used as an input to the model is determined empirically using an alternative empirical model geometry (e.g. a sphere). Details of the parameterization of the model are outlined in Holmgren (2013). The model is driven by a combination of internal diffusion (D) based on Fick's first Law and the empirical Piringer equation (Piringer and Baner, 2008), material-specific equilibrium partitioning coefficients ($K_{M/A}$) and convective mass transfer coefficients (h_m) using a boundary layer model for flows over planar surfaces (Welty et al., 2010).

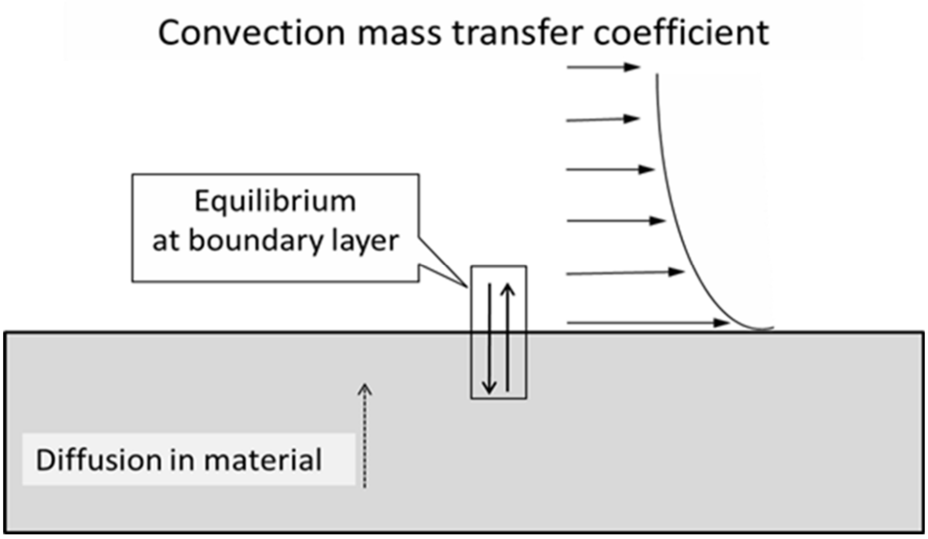
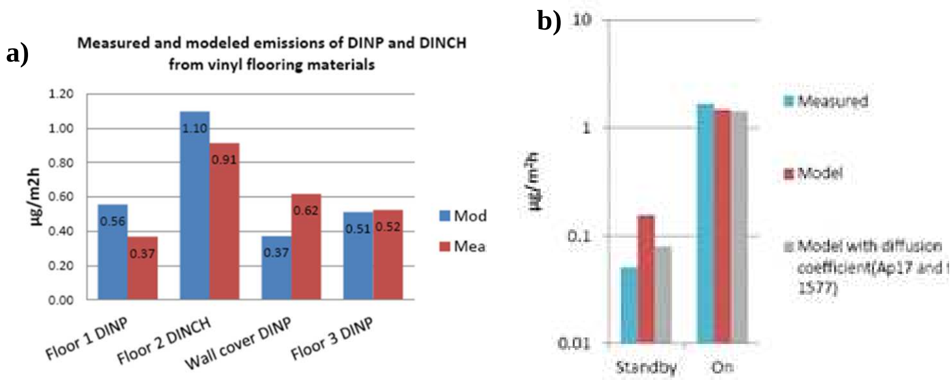


Figure 0-10. Illustration of the ChEmiTecs mechanistic emission model.

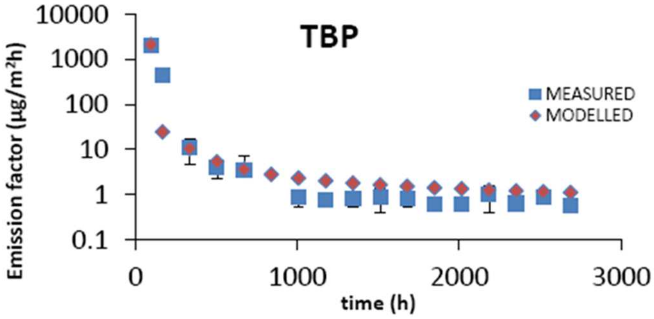
To improve the underlying data used in the development of the ChEmiTecs emission model and to provide data for model evaluation, experimental studies of emission mechanisms from case study articles were undertaken (Cousins et al., 2014; Holmgren, 2013; Holmgren et al., 2013a; Holmgren et al., 2013b), which considered:

- emissions to indoor air from vinyl flooring
- emissions to indoor air from flat-panel LCD-screens
- leaching to water of tributylphosphate (TBP) and triisobutylphosphate (TiBP) from concrete

The results from the measurements were compared to model predicted emission rates in order to evaluate the model accuracy and showed generally good agreement (Figure 0-11), illustrating the general functionality of the model, if the specific use conditions are known. The current version of the emission model was less accurate for multilayer materials such as polyurethane covered PVC-flooring materials, where emission rates are reduced due to additional diffusion barriers.



c)



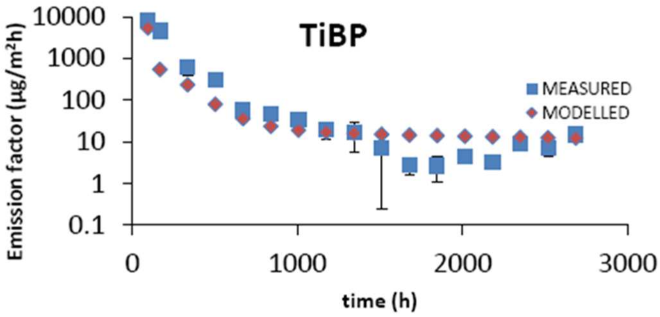


Figure 0-11. Comparison between model predicted emission rates using the advanced emission model and experimental emission rates of a) DINP and DINCH from vinyl floors b) TPP from flat panel displays and c) TBP and TiBP from concrete.

The model was used to predict national emissions of five different additives from vinyl floors to indoor air (in a standard room environment) during the time period between 1990 and 2035 based on sales statistics, an assumed plasticizer content of 16 % and an assumption that future annual sales data would be the same as in 2010 (Figure 0-12). As the figure shows, emissions of DEHP have decreased steadily since 1990 due to gradual phase-out from new products. The remaining emissions are a result of the long service life (20 years) of PVC-floors, and emissions are expected to have ceased around the end of this decade. A replacement with DINP or DINCH was predicted to lead to much lower emissions, whereas some of the other potential replacements are expected to lead to higher emissions, despite the assumption of equal chemical content. This example illustrates the influence of molecular properties on the emission strength from a certain product.

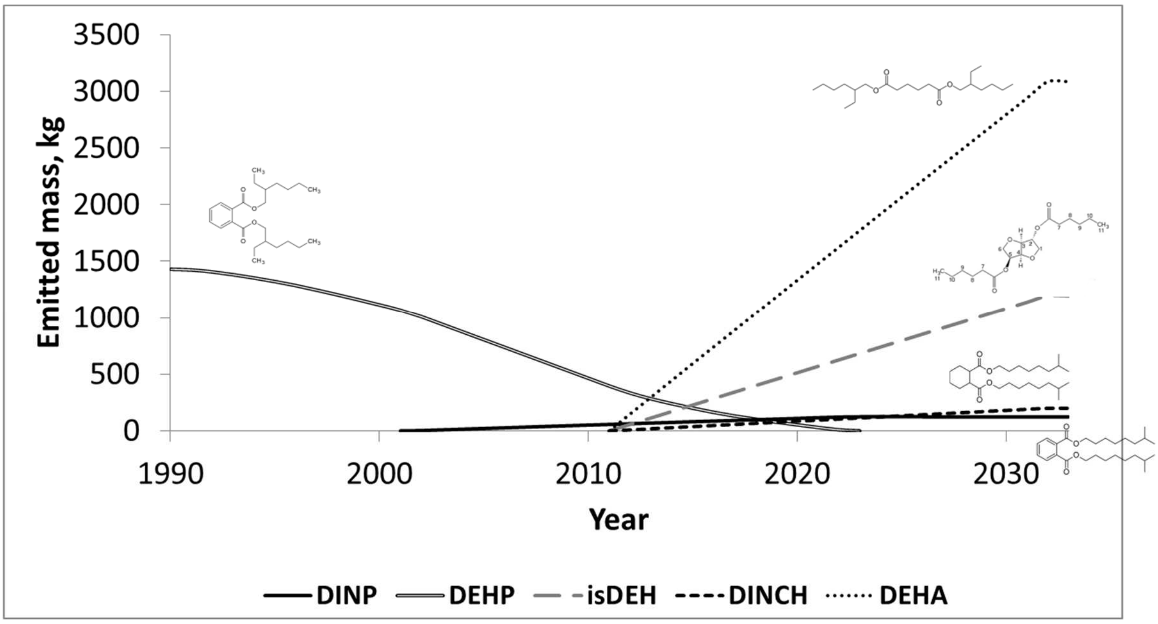
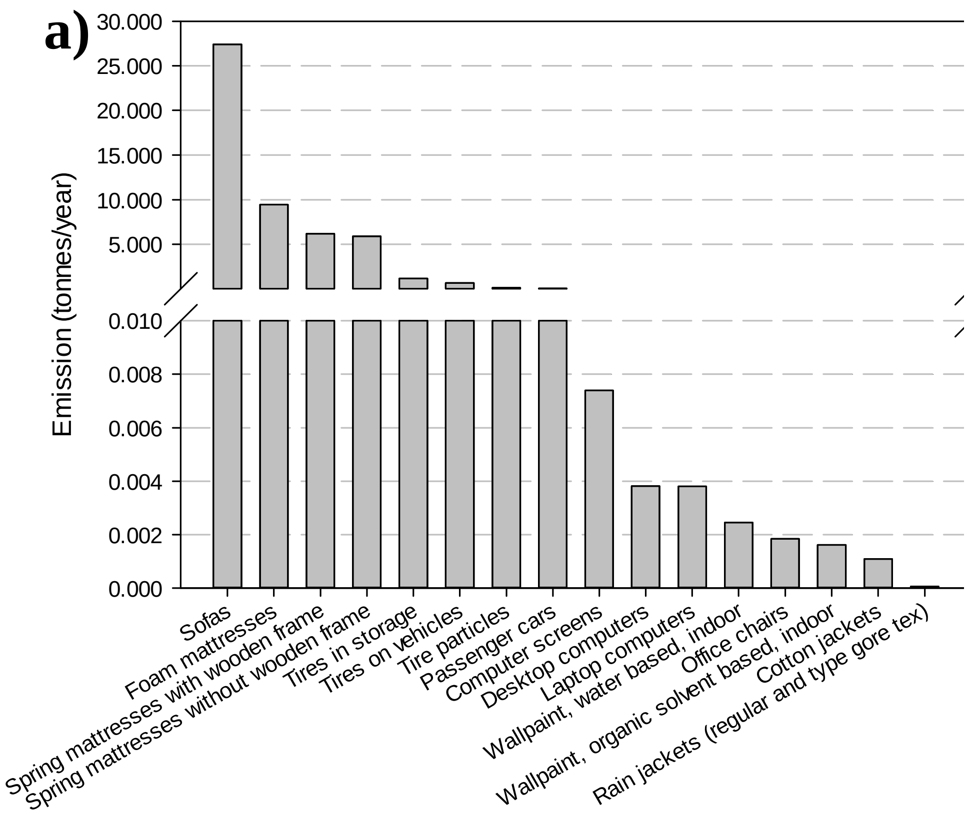


Figure 0-12. Estimated emissions of plasticizers from vinyl flooring. DINP: diisononyl phthalate
DEHP: diethylhexyl phthalate, isDEH: dietylhexyl isosorbate DINCH: Cyclohexandicarboxylic acid diisononyl ester DEHA: Dietylhexyl adipate. Adapted from (Holmgren et al., 2012)

As a next step, the ChEmiTecs Emission model was applied to additives incorporated in the case study related product categories illustrated in Figure 0-6. The most important product categories from an emission perspective were upholstered furniture such as sofas and mattresses followed by tires and passenger cars whereas all other selected product categories appear to be of less importance (Figure 0-13a). From a chemical perspective, the mechanistic emission model predicts highest emissions of melamine followed by TCPP and triethylphosphate. The predicted overall emissions from the case study product categories amount to **51 tonnes/year**. Melamine was predicted to be the most predominant substance emitted, followed by triethylphosphate, TCPP, resorcinol, styrenated phenol, 4-nitrophenol, diphenylamine, 2-naphthylammonium acetate and 3,5-dichloro-(1,1,2,2-tetrafluoroethoxy)-aniline, accounting for 97 % of the emissions of the 415 chemical substances included in the assessment (Figure 0-13b).

4.3.3 Indoor vs outdoor emissions

Based on the knowledge and assumptions of use patterns it can be concluded that a large part of the emissions are directed towards the indoor environment. The chemicals occur in the wide category of products that includes building materials (flooring, paint, wallpapers, varnish etc.), furniture and textiles and electronics. Therefore many of the chemicals are likely to undergo indoor fate processes which will influence the potential for human exposure as well as their further transport to the outdoor environment as illustrated in Cousins (2012). This may include direct transport to the outdoor environment via ventilation outlets or indirect transport via sewage systems (e.g. washing of clothes), but may also lead to ultimate removal via incineration (due to combustion of vacuuming bags and household waste), or recirculation via waste recycling systems. Some emissions are however directed towards the outdoor environment directly, e.g. via plastic tubing and roofing materials and the wear and tear of shoes, tires and outdoor tarpaulins.


a)
Emission (tonnes/year)
30.000
25.000
20.000
15.000
10.000
5.000
0.010
0.008
0.006
0.004
0.002
0.000
Sofas
Foam mattresses
Spring mattresses with wooden frame
Spring mattresses without wooden frame
Tires in storage
Tires on vehicles
Tire particles
Passenger cars
Computer screens
Desktop computers
Laptop computers
Wallpaint, water based, indoor
Office chairs
Wallpaint, organic solvent based, indoor
Cotton jackets
Rain jackets (regular and type gore tex)

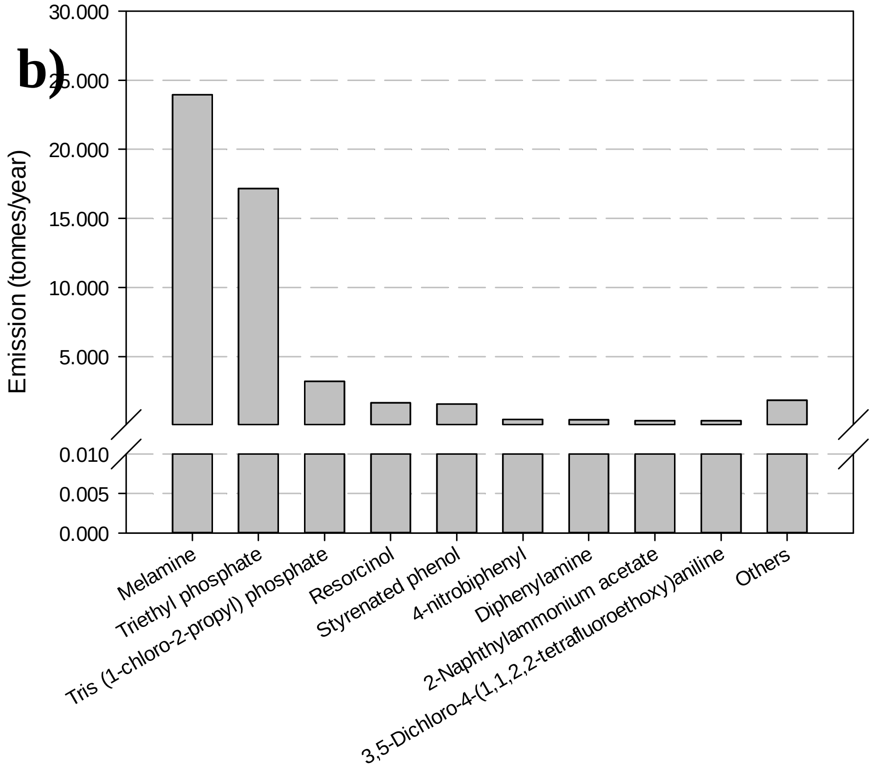


Figure 0-13. Estimated annual emissions of a) chemical additives from 16 selected product categories in use and b) 10 dominant organic chemicals from 16 selected product categories.

Again, there is no linear relationship between estimated stock and estimated emissions calculated using the ChEmiTecs emission model. With the exception of 1,3-benzenediol and styrenated phenol, the estimated emissions are low compared to the estimated stocks, which is also illustrated in Figure 0-14.

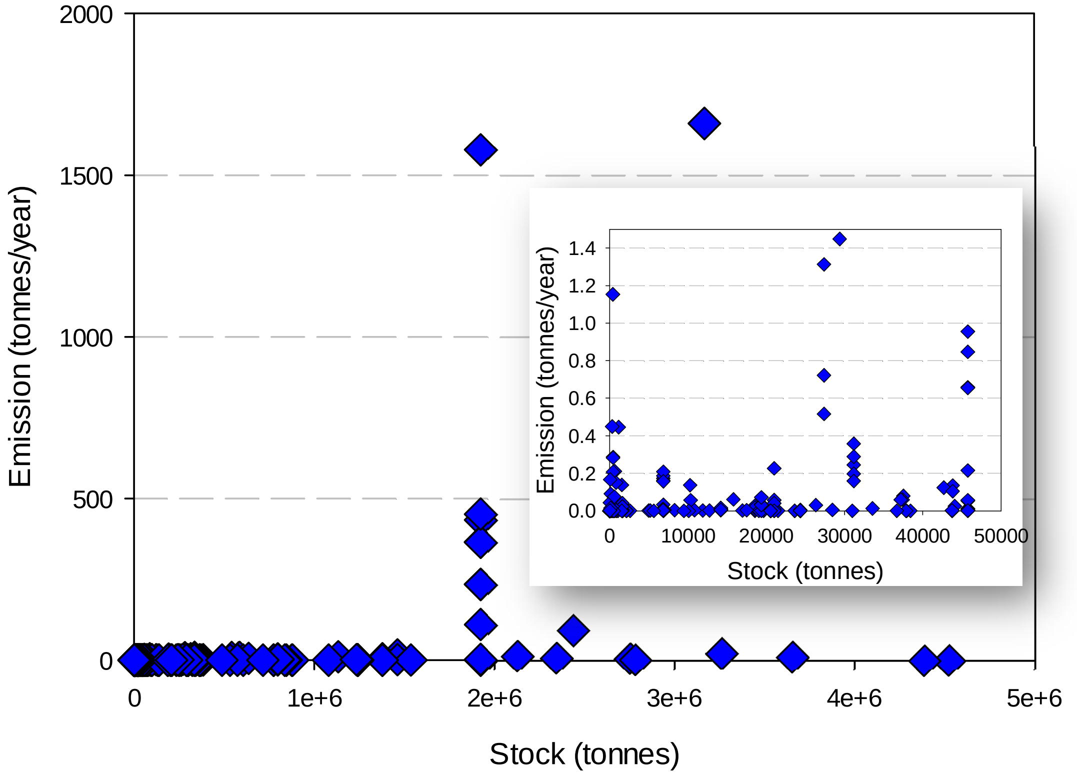


Figure 0-14. Relationship between estimated stocks and estimated emissions of chemical additives in 16 selected product categories. The small inserted picture shows emissions between 0 and 1.5 tonnes/year.

4.4 Estimated remainder of additives at article end-of-life

To estimate the remainder of chemical additives in consumer articles at end-of-life, annual emissions were multiplied by the service-life of each article category and subtracted from the calculated chemical stock of that article category. This is a conservative approach in that it assumes that the emissions from a certain "article batch" are identical each year during the article lifetime and neglects the fact that emissions may be reduced with increasing article age. For all of the article categories over 99 % of the additive amounts are expected to remain in the articles at the end-of-life. Thus the majority of chemical additives applied in consumer articles are expected to follow articles into the waste and recycling phase.

4.5 Top-down approach to estimate emissions: inverse chemical fate modelling

Within ChEmiTecs, an indoor-inclusive urban fate model (SMURF) was developed (Cousins, 2012) and used to back-calculate emissions of DINP, DEHP and BDE 209 to indoor air in the city of Stockholm using experimental data on indoor air and dust

(Cousins et al., 2013). The model was further used to estimate article-related emissions to indoor air of case study chemicals (Cousins et al., 2015), assuming that articles are the dominant sources of these chemicals in the indoor environment, and estimates were up-scaled to the national level using the population ratio between Stockholm and Sweden. Estimated emissions to Swedish indoor air were 40, 580, 300 and 11 kg/year for DINP, 8:2 FTOH, TBP and TPP (Cousins et al., 2015). Emissions of MBT and diuron could not be estimated due to lack of monitoring data in the indoor environment.

4.6 Comparison of methods

Comparing the two bottom-up approaches reveals that the relationship between estimated stocks and emissions differs between the two methods applied. Whereas the OECD approach results in the emission:stock relationship 50000:3000000 or 1:60, the ChEmiTecs approach generates the corresponding relationship of 51:310000 or 1:6000. Acknowledging the fact that the ChEmitecs approach was conducted at a higher level of detail, assessing articles and chemicals of high representability of the overall societal stock and to some extent verified using empirical measurements we argue that the latter estimate presents a relationship, which is likely to be more representative of the reality, i.e. that the OECD model overestimates the emissions by a factor of 100. This would imply that the real emissions of plastic additives lie around **500 tonnes per yea**r, which is the value used in the further assessments. This figure applies to parent substances, i.e. *does not consider potential emissions of transformation products*. To evaluate the comparability of the estimation methods further, article-related emissions were calculated for six specific chemicals using the three methods described above (Figure 0-15). As evident from the figure, different methods result in different emission figures, but the OECD emission model generally overestimates the emissions compared to the other methods used. The inverse modelling compares well to the estimated emissions of DINP and TPP to indoor air using the ChEmiTecs emission model, which were mainly estimated based on PVC floors and flat panel displays. This is interpreted as an indication that these article categories are important source categories in the indoor environment. All methods have their advantages and disadvantages, thus it is clear that the emissions are best assessed by combining different methods.

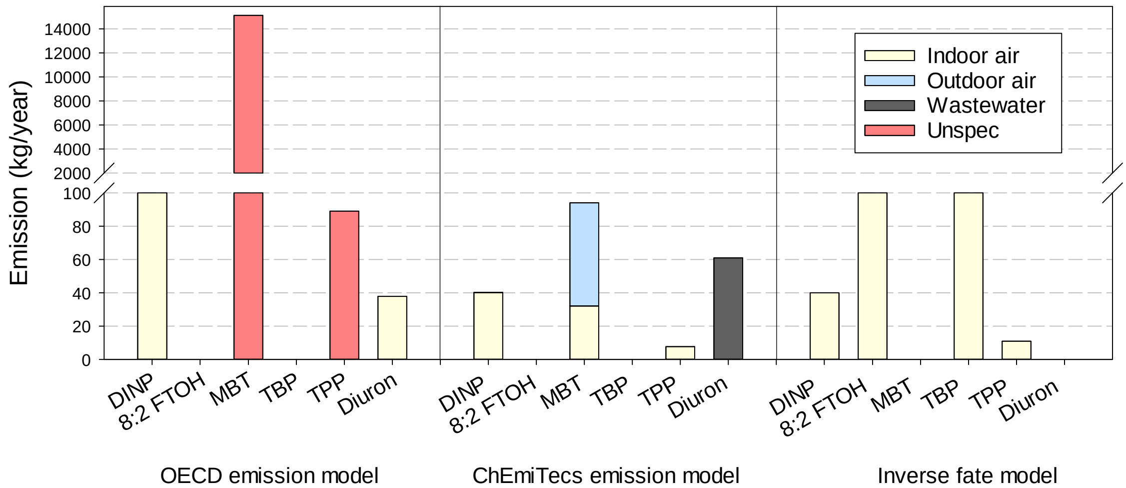


Figure 0-15. Estimated article-related emissions of case study chemicals using three different modelling approaches.

It should be emphasized that the estimated emissions concern molecular emissions of parent compounds (i.e. not transformation products), whereby e.g. tire particles are considered to be a separate article with a specific surface area from which molecular releases can occur. Thus, an abraded particle transported to wastewater or air is not considered as an "emission" in this sense but as a transport vehicle for molecules which may later be emitted through molecular diffusion (see chapter 2.4). As such these are also included. Other studies have estimated the abrasion of tire particles to be in the order of 10 000 – 13 000 tonnes/year (Magnusson et al., 2016; Norén and Naustvoll, 2010), which would then carry with them approximately 1000 tonnes of additives which could potentially be released through molecular mechanisms (assuming an additive content of 10 %). A recent study investigated the environmental release of additives and their transformation products from tire particles during different lifecycle stages (manufacture, TRWP generation (wear) and environmental release) (Unice et al., 2015). The total fraction released to the environment (water and sediment) were estimated to be 6 to 10% of the formulation mass, depending on the substance and the age of the particle, again indicating that chemical properties are important drivers of emissions from articles. Applying these fractions to the estimated particulate release of tire particles in Sweden generates an estimated molecular environmental release of tire additives between 60 – 100 tonnes, i.e. 12 – 20 % of the total estimated additive emissions by ChEmiTecs. This, however, includes also transformation products, which were not included in the ChEmiTecs approach. Again this emphasizes the need to apply different, independent methods to estimate emissions, which combined can build up a stronger knowledge base on actual chemical emissions to the environment.

5 Are emissions from articles of concern?

5.1 Summary and recommendations

The various studies conducted within this program indicate that from a general perspective, emissions from articles cannot fully explain the environmental occurrence of the substances, thus other emission processes, sources and pathways such as particulate emissions, material-dust partitioning, industrial releases and atmospheric long-range transport may also be important. However, when it comes to the indoor environment, consumer articles are dominant sources of many organic chemicals, and may thus have a significant contribution to human exposure. Thus special attention should be drawn to the indoor environment, where people spend the majority of their time. Special focus should then be drawn to chemicals present in porous materials and high molecular diffusivity.

According to the surveys conducted within the program with consumers and producers, emissions from articles are not generally perceived to be of major concern. Producers are of the opinion that they have the necessary tools to perform risk assessments, and they are reasonably content with the current legislation. Legislation is viewed as the main driver in the environmental work whereas the national environmental goals do not have a major influence. Consumers are mostly concerned with potential risks for workers and to the local environment near production plants. In general, consumers prefer labelling as a way of communicating article contents.

A comparison with biocides, based on a potential ecotoxicity calculation model from the life cycle assessment domain, indicates lower overall potential ecotoxicity of emissions of chemical additives from plastics compared to potential ecotoxicity associated with intentionally released biocides on the national Swedish scale. However, the end-points used do not cover all potential effects, and due to data gaps it was not possible to assess the potential ecotoxicity of all additives. In general, too little is known about the properties and toxicity of chemical additives in consumer articles, which complicates the possibility to thoroughly evaluate the importance of emissions from articles from a risk perspective.

Our studies indicate that technosphere articles are major sources to DINP and TPP indoors, illustrating the importance of the indoor environment as a primary recipient of chemicals in articles. The occurrence of a substance in the indoor environment does not automatically imply that there is a risk, but the knowledge of the potential for build-up of higher concentrations indoors illustrates the need for special attention to be paid to articles aimed for indoor use. We therefore urge product developers to pay special attention to chemicals incorporated in articles made of porous materials of large surface areas, aimed for use in the indoor environment. Since these types of articles are most likely to emit largest amounts of additives, and

cause relatively high indoor concentrations it is important to ensure that chemicals incorporated in such articles are safe.

5.2 Properties of Chemicals of concern

5.2.1 Chemical Stability and Bioaccumulation

The concepts "Persistence" (P) and "Bioaccumulation" (B) are essential for describing the fate of chemicals in the environment. The term "persistence" refers to the chemical's ability to withstand chemical reactions: "*The persistence of a chemical is its longevity in the integrated background environment as estimated from its chemical and physico-chemical properties within a defined model of the environment*" (Green and Bergman, 2005). The chemical reactivity has a strong influence on persistence, in parallel to the physico-chemical characteristics of the compound. A highly stable chemical, only undergoing very slow transformations under abiotic conditions, is available for partitioning in the environment for a very long time, and will do so according to its physico-chemical partitioning properties. These depend on the chemical's ability to undergo molecular interactions with the surrounding environment (affecting e.g. water solubility, volatility etc.). Bioaccumulation is dependent on two major properties of the chemical species; its reactivity in biota, i.e. its susceptibility to be metabolized, and it's partitioning to and within the organism.

Several types of reactions are at stake when studying reactivity: *hse*-reactions (hydrolysis/substitution/elimination), oxidations, reductions, direct photolysis and reaction with radicals. In studying the environmental fate of chemicals, different reactions are relevant for different chemicals and in different phases of the fate and transformation process. Table 0.5 displays selected chemicals relevant in the ChEmiTecs project and an indication of their reactivity.

Table 0.5. Selected chemicals and an indication of their chemical reactivity (Based on (Eriksson and Bergman, 2010)

Substance (group)	Reaction to which the chemical is susceptible	Reaction to which the chemical is not (very) susceptible	Other aspect
Phthalate esters	Free radical reactions	Photolysis, oxidation, reduction	Readily transformed biologically
Phosphate esters	Free radical reactions	Photolysis, oxidation, reduction	Readily transformed biologically
Brominated diphenyl ethers	Reduction	N.A.	N.A.

In a study looking specifically at properties of chemicals often used in articles, it was found that 25 chemicals (in 14 chemical groups) of the 101 most used in articles in Sweden were problematic in terms of PB-properties (Almqvist, 2011). Six of these 101 chemicals are classified as Substances of Very High Concern (SVHCs) by the European Commission, two are included in the Stockholm Convention as Persistent Organic Pollutants (POPs), seven are classified as persistent and/or bioaccumulating by the European Commission, two are included on the SIN List, two are regarded as persistent and/or bioaccumulating by other reliable sources and eight structurally resemble substances that are known to be persistent and/or bioaccumulating. All of the chemicals that are or may potentially be persistent and/or bioaccumulating are organic compounds and most of these are halogenated.

5.2.2 Toxicity

An initial data search was carried out during the first half of the ChEmiTecs program, aiming to identify studies investigating the toxicity and or ecotoxicity of prioritized compound groups (benzenediamines, benzothiazoles, benzotriazoles, organophosphates, PFCs and DINP) (Molander, 2010). For several of the substances in the groups, data were not available in scientific literature. Although this can be expected, it nevertheless points at a challenge for research in the area. In an experimental study within ChEmiTecs, the toxicity of wear particles from shoe soles was studied. The shoe soles were abraded and leached in water for 29 days and the alga *Ceramium tenuicorne* and the crustacean *Nitocra spinipes* were exposed to different concentrations of the leachate. Chemical analyses were performed to determine the chemical contents of the leachate. The main conclusions were that the shoe soles contain substances that are toxic to both test organisms, and that the toxicity is mainly explained by the presence of zinc (Ingre-Khans et al., 2010). Thus the organic substances present in the shoe material were not the main eco-toxicity issue, although a parallel study on the content of organic chemicals in shoes revealed a range of potentially hazardous substances (Dahlberg, 2010). Three compounds found (diisobutyl phthalate, dibutyl phthalate and bis(2-etyhylhexyl)phthalate) are included on the candidate list for authorization within REACH. However, the levels were approximately 100-1000 times lower than the limit stated in REACH (Dahlberg, 2010).

5.2.3 Estimating properties based on structure

For several decades, computational methods have been developed and used to estimate physico-chemical as well as other (e.g. fate and toxicity related) properties of substances including read-across, trend analysis, Quantitative Structure-Property Relationships (QSPRs) and Quantitative Structure-Activity Relationships (QSARs) (Furusjö et al., 2001). These approaches are based on the concept that the these properties of substances are determined by their chemical structure. In ChEmiTecs, these approaches have been useful in several chemical selection and modelling steps to fill data gaps and evaluate large numbers of chemicals,

- for the prioritization and selection of chemicals for case studies (Rännar and Andersson, 2010),
- for identification of possible gaps in legislation (Molander et al., 2012a),
- for the development of the generic emission model (Holmgren et al., 2012; Holmgren 2013) as well as in the fate modelling (Cousins, 2013) and
- for the risk estimation of additives in relation to biocides in a life cycle impact assessment approach (Palm, 2014).

5.3 How large are the emissions from articles in comparison to emissions from other sources?

To address this issue, two parallel approaches were used, which are briefly described below:

a) Substance Flow Analysis (SFA), whereby estimates of nationwide emissions from consumer articles (se chapter 4) were compared to emissions from other sources and pathways, such as industry and atmospheric deposition, estimated using SFA methodology (Figure 0-16).
b) Multimedia fate modelling, whereby estimated emissions from articles and municipal wastewater treatment plants (M-WWTPs) were scaled to the Stockholm level and used as input to the SMURF model (Cousins, 2012). Model predicted environmental concentrations were compared to monitoring data from Swedish databases to find out if emissions from articles and M-WWTPs may explain the concentrations found in the environment (Figure 0-17).

An initial literature study (Paulsson, 2010) revealed a severe scarcity of environmental data of target compounds in the scientific literature. To provide additional monitoring data to allow for comparison between modelled and measured concentrations, a separate environmental screening study was conducted for benzotriazoles and benzothiazoles (Brorström-Lundén et al., 2011). The benzothiazoles MBT, CBS, DBS and DBD were all found in one or more of the matrices sampled.

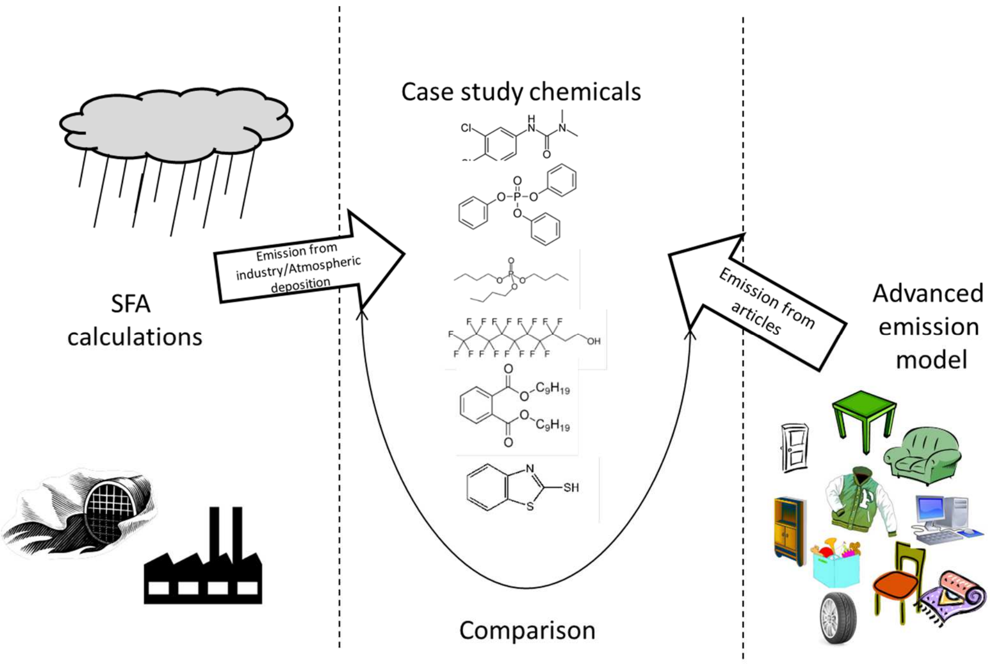


Figure 0-16. Evaluating the importance of article-related emissions using SFA methodology.

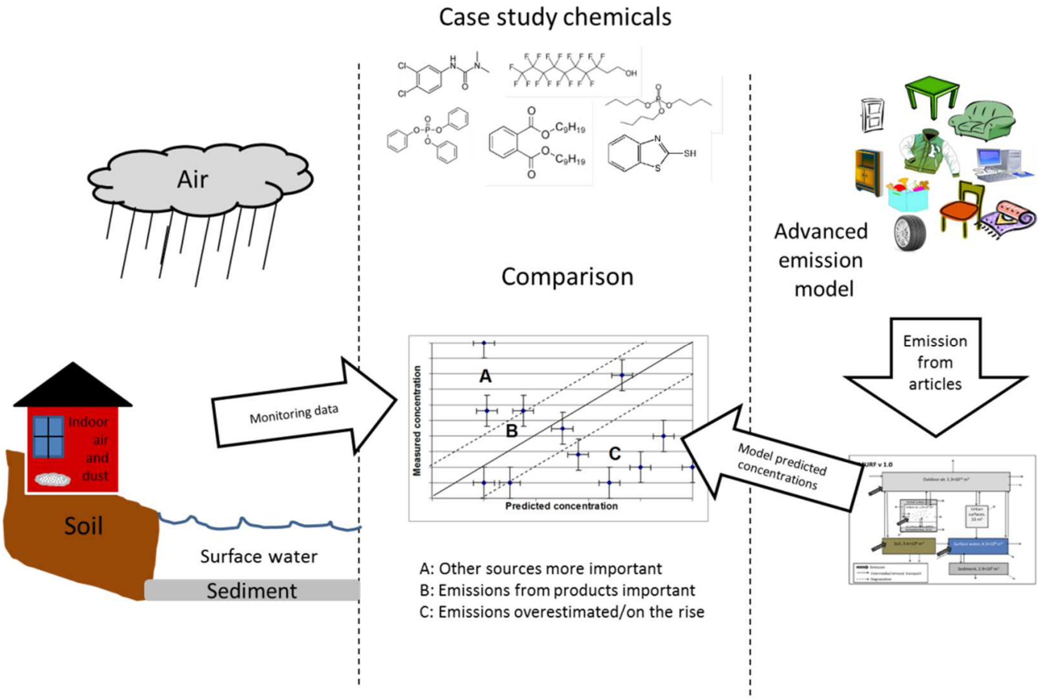


Figure 0-17. Evaluating the importance of article-related emissions using monitoring data and the SMURF model.

Overall, the relative importance of emissions from articles appears to depend on the substance as well as on the primary recipient, i.e. the mode of release. It is therefore not possible to give a clear answer to the general question "Are emissions of organic substances from articles more important than emissions from other sources?" However, for the case study substances, emissions from articles appear to be lower or in the same order of magnitude as other sources, such as industrial emissions. For most of the studied substances, emissions to the indoor environment are dominated by emissions from articles, thus concentrations found in ***indoor air and dust*** can largely be explained by release from articles, which is very relevant in terms of human exposure. For some substances (e.g. for TBP and 8:2 FTOH), ***occurrence in outdoor air*** can to some extent be explained by estimated emissions to indoor air, i.e. emissions from consumer articles. Urban soil data were generally scarce for the substances assessed, but the ***occurrence in the aquatic environment*** is generally ***not explained by emissions from consumer articles*** only (Cousins et al., 2015).

5.4 Risk perception among consumers and producers of articles

Few studies have focussed on the perception of risks associated with chemicals emitted from consumer articles on the general population. Two separate surveys were undertaken within ChEmiTecs, one focussing on how producers perceive and act when it comes to potential risks with chemicals in the goods they produce (Wester, 2012b), and one focussing on the perception of risks of different consumer goods among the Swedish public (Wester, 2012a). The studies were undertaken as telephone interviews with a total of 101 producers and as a national survey with 2000 consumers and focussed on five article groups, selected from the identification of case studies: *i)* Electronic goods, *ii)* Tyres, *iii)* Textiles, *iv)* Shoes and *v)* PVC flooring. The interviews with the producers covered ten sections regarding risk assessment, communication and risk perception. The consumers were asked questions regarding risk perception and information preferences. The results indicate that producers have access to the information needed in order to perform reliable risk assessments; have a good communication with their customers, and are content with the current regulation of chemicals. The national goal of a “non-toxic environment” is not used to a large degree, thus the relevance of this goal for industry appears to be limited. From the consumer perspective, risks to the environment from chemical pollution are seen as greater than risks to health, and risks are perceived to be greatest for the local environment and to the workers where production of these articles takes place. Knowledge of what different labels on consumer articles stand for is high and labels are a preferred way of receiving information about an article.

5.5 Risk estimation in relation to biocides

The underlying concern with any chemical releases is the potential for negative effects on human health or the environment. Although the main focus of ChEmiTecs has been on the content and emissions of chemicals in and from articles, the ultimate goal for any regulation policy is to reduce and/or avoid risks associated with chemical exposure to humans and wildlife. For this reason, a “chemical footprint approach” was undertaken (Rydberg et al., 2015), whereby risk scores were calculated using UseTox characterisation factors (CFs) (Rosenbaum et al., 2008) and estimates of stock and emissions of plastic additives in Sweden using the OECD emission approach (Rydberg et al., 2012). The results were compared to the corresponding risk scores for biocides, again using UseTox CFs and national consumption data for biocides from 2012 (KEMI, 2013). Because of the lack of CFs for the additives of concern, a separate study was undertaken to fill the data gaps (Palm, 2014). This generated a total of 90 CFs out of 215. The resulting estimated risk scores are shown in Table 0.6, indicating that the risk (based on freshwater toxicity) associated with emissions of additives from plastics is somewhat higher than the estimated risk from biocides. Bearing in mind, however, that the OECD model was observed to overestimate emissions from articles by approximately a factor of 100 (see 4.6), a more realistic estimation is that the risk from biocides is about 1-2 orders of magnitude higher than the risk associated with additives from plastics, acknowledging the fact that the CF coverage for additives (42 %) was lower than for biocides (65%). This assessment gives an indication about the potential risk level of chemicals emissions from articles, in relation to another group of substances which are deliberately released into the environment. It should however be acknowledged that the current risk characterisation does not take into account all possible ecotoxicological end-points neither of the additives nor of the biocides.

Table 0.6. Estimated risk score of chemicals in and released from consumer articles compared to estimated risk scores for biocides, using a chemical footprint approach (Rydberg et al., 2015).

	Chemical additives in plastics (see chapter 3.2), OECD emission model (chapter 4.3.1)		Chemical additives in 16 case study articles (see 3.3), ChEmiTecs Emission model (chapter 4.3.2)		Biocides in Sweden (KEMI, 2013)
	Stock	Estimated annual emissions	Stock	Annual emissions	Annual consumption
Total amount (tonnes)	**2700000**	**47000**	**310000**	**51**	**9200**
Amount of chemicals used for risk characterisation (tonnes)	1240000	29300	170000	47	1300
Risk score ($PAF/m^3/day$)*	**9.2×10^{11}**	**3.1×10^{10} a,b)**	**1.3×10^{10}**	**2.3×10^{5} c)**	**9.3×10^{9}**

*)CF as freshwater toxicity through emissions to continental rural air, PAF = potentially affected fraction (Rosenbaum et al., 2008)

a) of which CAS:133-07-3 ("Folpet"), 83 %; and CAS: 118-79-6 (2,4,6-Tribromophenol), 8 %

b) the estimate is believed to be overestimated by a factor of about 100

c) of which CAS: 108-78-1 (Melamine); 58 %; and CAS:13674-84-5 (TCPP), 10 %

6 Risk reduction strategies

6.1 Summary and recommendations

The research conducted within ChEmiTecs indicates a need to strengthen product specific legislation as a complement to REACH to mitigate chemical risks for certain articles, e.g. building products and textiles. The research also recommends that the prioritization of chemicals to be regulated in articles under REACH to a greater extent takes into account substances that have been identified as posing a risk to the environment. The substitution principle stipulates that if risks can be reduced by replacing a chemical, mixture or product by some other technology, this should be done.

One of the most efficient ways to change consumption patterns are through voluntary agreements, as they come into force as soon as the agreements have been settled. It is also possible for market actors to be more progressive than the law demands through voluntary agreements. A pre-requisite for such agreements to take place is that there is a consumer pressure, which requires well-informed and motivated consumers. The role of voluntary agreements is exemplified with BASTA, the Swedish building industry's own initiative to phase out hazardous chemicals, which is frequently used as requirements in public procurement. The studies showed that the Swedish environmental goals are not important drivers towards voluntary agreements to reduce chemical contents in consumer articles.

The ChEmiTecs studies strengthen the position of the Swedish Chemicals Agency that legislators should consider developing product specific rules such as those exemplified by the RoHS and the WEEE directives, as a complement to the REACH rules that target the use of chemicals in articles.

6.2 Risk reduction through legislation

The role of the European chemicals legislation and the suitability of current legislation to manage health and environmental risks associated with chemicals in articles have been studied in a series of papers and presentation (Molander et al., 2012; Molander et al., 2011; Molander and Rudén, 2012) included in a licentiate thesis published in 2012 and later on in a Ph D thesis respectively (Molander, 2012; Molander, 2015). A comparison of different EU regulatory frameworks targeting the use of chemicals in articles identified a number of shortcomings and inconsistencies in how chemicals in articles are regulated. It was concluded that to ensure adequate control of health and environmental risks of chemicals in articles, the development of product-specific rules, such as those exemplified by the RoHS and the WEEE directives, should be considered for articles currently only regulated by REACH and which are widely used and known to include hazardous chemicals (Molander and Rudén, 2012). It was further suggested that the use of chemicals in articles could constitute a possible obstacle for meeting environmental goals (Molander et al., 2012a). More specifically, it was shown that the majority of the chemicals or groups of chemicals that were prioritized for phase-out under the Water Framework Directive or for concentration restrictions in sludge and soil under the Sewage Sludge Directive were allowed for use in articles according to REACH. It was therefore recommended that the prioritization of chemicals to be regulated in articles under REACH to a greater extent should take into account substances that have been identified as posing a risk to the environment.

The SU/KTH research group has continued to work with issues aiming to contribute to improving the management of chemical risks also after the end of the ChEmiTecs project. The work includes the development of a method for systematic and transparent evaluation of *in vivo* toxicity studies, which aims to facilitate the use of non-standard research studies and fill information gaps in health risk assessment. The evaluation method is available online at http://www.scirap.org/ (Molander, 2015).

6.3 The substitution principle

Within chemicals regulation and risk management, *the substitution principle* is a policy principle aimed to replace harmful substances by less harmful alternatives. The interpretation and applicability of this principle has varied between different groups of appliers, and ChEmiTecs researchers identified a need for clarifying the meaning of this policy principle, and to suggest conditions for implementation of the principle. These issues are outlined in Hansson et al. (2011). The following definition of the substitution principle was proposed:

> *"If risks to the environment and human health and safety can be reduced by replacing a chemical substance, mixture or product or by some non-chemical technology, then this replacement should be made. All decisions on such substitutions should be based on the best available evidence. This evidence can be sufficient to warrant a substitution even if it only consists of hazard information and quantitative risk estimates cannot be made"*

In Hansson et al. (2011), examples of methods to promote substitution are presented, and it is discussed how the choice of methods can and should be performed in order to be an effective tool for reducing chemical risks associated with consumer articles. It is stated that the primary responsibility for avoiding hazardous substances and processes rests with the chemical industry.

6.4 Risk reduction through voluntary initiatives – the example BASTA

The ChEmiTecs research program included an exemplification on how voluntary agreements may be used to reduce risks associated with chemicals in consumer articles. This work has been carried out in association with the existing BASTA-system, a voluntary initiative from the building industry to phase out hazardous substances www.bastaonline.se. BASTA is successfully used by the building industry to avoid hazardous substances in building products and currently (March, 2016) includes 96 000 individual building products that fulfil the requirements regarding environmental and health hazards. By registering their product in BASTA, the company guarantees that their product does not contain any chemicals with properties given by the BASTA criteria. In collaboration with BASTA, the ChEmiTecs researchers have expanded the BASTA system to include a risk module by adding a so called BETA register to the existing BASTA system, that would allow companies to register products that do not fulfil BASTA criteria but may still be accepted from a risk perspective (Green, 2009; Jarnhammar et al., 2008). The risk module that was developed included the following parts:

- Property Criteria for products in BETA database.
- Completing terms for vendors with products in the BASTA and/or BETA
- Documents of requirements for risk information for BETA-registered products
- Completing a routine for validation
- Completing a manual for suppliers
- Completing template for subcontractor declaration
- Supplementation of IT tools for registration and enforcement of BETA-registered products
- Development of sales and information in the form of a newsletter.

All documents, including the BETA register are available online at www.bastaonline.se.

7 Conclusions

The work conducted during the five years of the research program has led to increased insights regarding the extent and scale of the problem of emissions of organic chemicals in articles, and in the identification of remaining challenges associated with the issue.

Regarding the total accumulated **stocks** of chemicals in technosphere articles, it was concluded that:

- The total stock of organic chemical additives in plastic materials in articles used in Sweden is estimated to **3×10^6 tonnes.**
- Product categories where large amounts of chemical additives are stored are pipes and hoses, plastic products such as films and boards, insulated wires and cables, furniture (sofas), passenger cars including tires.
- Chemicals stored in large amounts are typically plasticizers (phthalates and adipates) organic pigments and flame retardants, but also substances such as melamine, rapeseed oil and stearic acid.
- Only a minority of the additives incorporated in products are expected to be released during the use phase, more than 99 % of additives are expected to remain in consumer products at the end of their lifetime.
- The general lack of information of chemical content in articles presents a significant obstacle to obtain reliable estimates of chemical stocks and thus reliable estimates of chemical flows into the waste stage.

Concerning the **emissions**, the following conclusions were drawn:

- Emissions of organic chemical additives from plastic materials in articles used in Sweden are estimated at **500 tonnes/year.** This figure concerns parent compounds only, i.e. potential transformation products have not been included.
- The largest emissions during the use phase are likely to occur from products made from porous materials and materials with high surface area (e.g. upholstered sofas, passenger cars, car tires including abraded particles)
- Emissions are likely to be highest for additives with weak binding properties to the material matrix, which is associated with e.g. low molecular size and high volatility (i.e. low K_{OA}).
- Chemical groups of particular interest are plasticizers and flame retardants such as phthalate esters and organophosphates. Common for these substances are that many of the products they occur in are used in the indoor environment.
- For any given article, increased temperature may lead to increased emissions, e.g. of flame retardants from computer screens.
- Emissions from articles are best assessed by combining different estimation methods and should be cross-checked against empirical monitoring data.

When it concerns the **relative importance** of emissions from articles, the ChEmiTecs project identified that:

- Emissions from products via diffusion and indirectly via sewage treatment plants (which includes e.g. releases through washing of household textiles) cannot explain the outdoor environmental occurrence of the substances, thus other emission processes, sources and pathways such as gas and particulate emissions from combustion, industrial releases and/or atmospheric long-range transport may be equally or more important.

- Technosphere articles are major sources to DINP and TPP indoors, illustrating the importance of the indoor environment as a primary recipient of chemicals in articles. Due to the high number of articles used within small and confined spaces, which in general leads to higher concentrations compared to emissions outdoors, the indoor environment is of special interest.

The **perception** of the potential problems associated with chemicals in articles, as well as the general **availability of scientific knowledge** regarding their toxic properties was also addressed within ChEmiTecs and it was concluded that:

- Producers are of the opinion that they have the necessary tools to perform risk assessments, and they are reasonably content with the current legislation. Legislation is viewed as the main driver in the environmental work whereas the environmental goals do not have a major influence.
- Consumers are mostly concerned with potential risks for workers and to the local environment near production plants. In general, consumers prefer labelling as a way of communicating product contents.
- Data on properties and toxicity of additives in articles is largely missing in the scientific literature.

In addition to the conclusions drawn from ChEmiTecs, recent follow-up studies estimated the ecotoxic pressure from chemicals released from technosphere articles to be about 1-2 orders of magnitudes lower than the ecotoxic pressure from biocides. Recent research also indicates that direct migration to dust can contribute significantly to the levels found in the indoor environment.

Regarding potential **measures** it was concluded that:

- There is a need to strengthen product specific legislation as a complement to REACH to mitigate chemical risks for certain products, e.g. building products and textiles.
- One of the most efficient ways to achieve quick changes are through voluntary agreements within industry (exemplified by BASTA), but requires well-informed and motivated consumers.

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Emissions from Articles

Synthesis report of the ChEmiTecs Research Program

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Organic Chemicals Emitted from Technosphere Articles (ChEmiTecs) was a research programme funded by the Swedish EPA which ran during the years 2008-2013. The goal of the programme was to improve the understanding of mechanisms, magnitude and implications of emissions of organic substances from technosphere articles. It was also aimed at supporting the development of Swedish and EU management programmes to minimise risks from harmful substances. ChEmiTecs has been the first research programme to assess, on the National scale, the magnitude of the problem of emissions of chemicals in materials and articles.

The results now being published from the research programme are still of great interest both from a research- and from a policy perspective: For instance that even when accounting for article lifetime, normally more than 99 % of the added chemical additives remain in the products at the end-of-life, which means that the majority of the substances will enter the waste and recycling streams where they may be eliminated if the products are incinerated or re-circulated into new materials and products. Still, as the accumulated amount of additives is so large, the total molecular release to air of plastic and rubber additives from the total stock of articles in Sweden in the use phase during one year has been estimated to be in the order of 500 tonnes.

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