Assessing the relative importance of emissions from articles of selected organic substances

Anna Palm Cousins
Jenny Lexén
Katarina Hansson
Eva Brorström-Lundén

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ANNA PALM COUSINS
JENNY LEXÉN
KATARINA HANSSON
EVA BRORSTRÖM-LUNDÉN

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ChEmiTecs is a research program funded by the Swedish EPA. The program's goal is to improve the understanding of emissions of organic substances from articles and to clarify and determine the magnitude of this problem. The program aims to support development of Swedish and EU management programs to minimise risks from harmful substances. The program started in December 2007 and proceeded until September 2013. Participating organisations and organisation representatives are:

Swedish Environmental Protection Agency
(Funding organisation)
www.naturvardsverket.se

IVL The Swedish Environmental Research Institute Ltd
Tomas Rydberg (Programme manager)
tomas.rydberg@ivl.se
Eva Brorström-Lundén (Communications manager)
eva.bl@ivl.se

Stockholm University
Åke Bergman
ake.bergman@mk.su.se

Royal Institute of Technology
Christina Rudén
cr@infra.kth.se

Umeå University
Peter Haglund
peter.haglund@chem.umu.se

Chalmers University of Technology
Sverker Molander
sverker.molander@chalmers.se
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Extended summary

The aim of this study was to assess the importance of emissions of organic chemicals from articles in use compared to emissions from alternative sources, as part of the national research programme *Emissions of Organic Chemicals from Technosphere Articles* (ChEmiTecs). The assessment focussed on six selected case study chemicals: diisononylphthalate (DINP), triphenyl phosphate (TPP), tributyl phosphate (TBP), benzothiazole-2-thiole (MBT), 8:2 fluorotelomer alcohol (8:2 FTOH) and diuron. For these substances, emissions were estimated using two alternative strategies:

i. By comparing estimates of emissions from consumer articles (derived within the research programme) to emissions from other sources e.g. industrial releases and pathways e.g. atmospheric deposition obtained using substance flow analysis methodology (SFA).

ii. By comparing empirical monitoring data from urban Stockholm to predicted concentrations using a local-scale multimedia fate model (MEC/PEC). Physical-chemical properties were used as model input together with estimated emissions from articles and municipal wastewater treatment plants (M-WWTP). Where discrepancies were noted, backwards modelling was used to derive a likely emission scenario, based on monitoring data.

Overall, the relative importance of emissions from articles appears to depend on the substance as well as the receiving matrix. 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 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 emissions to indoor air, i.e. emissions from consumer articles. Urban soil data is generally scarce for the substances assessed, but the *occurrence in the aquatic environment* is generally not explained by emissions from consumer articles only.

The table below summarizes the findings for the case study substances using the two different assessment methods.
Assessing the relative importance of emissions from articles of selected organic substances

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Method i)</th>
<th>Method ii)</th>
<th>Estimated emissions in Sweden (method i and ii) kg/year*</th>
</tr>
</thead>
</table>
| DINP     | • Industrial emissions exceed emissions from articles by a factor of 400  
• Contaminated sludge is likely an important transport pathway  
• Atmospheric deposition potentially important pathway  
• Industrial emissions are likely to be decreasing due to a decreasing industrial use  | • Estimated emissions from articles to indoor air (4.1×10^{-6} kg/capita and year) explain the concentrations found in indoor air and dust  
• 200 and 800000 times higher emissions/background inflow to outdoor air and surface water are required to explain the levels in air and sediments respectively.  
• Monitoring data are lacking for soil, surface water and inflowing air | ![Graph showing emissions from different sources] |
| TPP      | • Industrial emissions are more important than releases from flat panel displays and upholstered furniture  
• Many important articles (e.g. hydraulic fluids) were missing in the assessment  
• Emissions from ‘all’ articles may be in the same order of magnitude as industrial emissions  | • Estimated emissions from consumer articles to indoor air (1.2×10^{-6} kg/capita and year or 11 kg/year in Sweden) explain the concentrations found in the indoor environment  
• The high estimated inflow with the atmosphere explain the occurrence in the urban atmospheric aquatic environment  
• Monitoring data are lacking for many matrices | ![Graph showing emissions from different sources] |
### Chemicals

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Method i)</th>
<th>Method ii)</th>
<th>Estimated emissions in Sweden (method i and ii) kg/year*</th>
</tr>
</thead>
</table>
| TBP      | - Assessment could not be completed due to missing data on industrial releases and very rough estimates from articles.  
- Leakage from hydraulic fluids, atmospheric deposition and release via M-WWTP effluents are potentially important transport pathways.  
- Emissions to indoor air estimated to $3.4 \times 10^{-8}$ kg per capita and year (or 300 kg/year) using backwards modelling.  
- Emissions to indoor air will be transported to outdoor air via ventilation.  
- Material abrasion and/or direct migration to dust is likely to be important release pathways, currently not captured in the assessment.  
- A background outdoor air concentration of 150 ng/m$^3$ is required to explain measured atmospheric deposition rates. | - General lack of monitoring data hinders a comparison between predicted and measured concentrations  
- Some evidence that current emissions to water are underestimated.  
- Estimated emissions to air resulted in higher predicted deposition rates than those measured  
- Estimated emissions therefore highly uncertain | ![Diagram showing emissions from various sources] |

| MBT      | - The assessment could not be completed due to missing data on industrial releases  
- Releases via M-WWTPs likely most important transport pathway, to which both industry and households contribute  
- Release from abraded tyre particles potentially important. | ![Diagram showing emissions from various sources] |
Assessing the relative importance of emissions from articles of selected organic substances

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Method i)</th>
<th>Method ii)</th>
<th>Estimated emissions in Sweden (method i and ii) kg/year*</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:2 FTOH</td>
<td>• Insufficient information for proper assessment.</td>
<td>• Lack of monitoring data for Sweden hindered a proper assessment • Using estimated emissions from a Swiss study ($6.0 \times 10^6$ kg per capita and year) and a background concentration of 0.014 ng/m³ resulted in predicted concentrations in indoor and outdoor air that agreed with measured concentrations in Norway and Canada, but an underestimation of dust levels.</td>
<td></td>
</tr>
</tbody>
</table>
| Diuron  | • Emissions of diuron from paint were estimated to 61 kg/year (mainly to wastewater). • Industrial emissions during manufacture are likely to be important. | • Estimated emissions from paint could not explain the concentrations found in the environment. • Sources other than painted walls and use of paint are likely to be more important for the environmental occurrence. | ![Graph showing emissions in Sweden](image)
Assessing the relative importance of emissions from articles of selected organic substances

In addition, the potential role of Stockholm as a source region to regional environmental pollution was assessed by comparing predicted incoming chemical amounts with outflowing amounts with air and water. The assessment indicated a potential contribution to regional pollution of the aquatic systems for MBT and diuron, whereas Stockholm appears to have negligible contribution to the surrounding environment for the remaining substances.

As indicated in the table above, large uncertainties were identified using both assessment methods and were mainly associated with lack of information on chemical composition of materials and lack of site-specific empirical monitoring data. It was therefore concluded that:

- 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.
- Empirical measurements (of emission rates and environmental concentrations) are needed at all stages in emission assessment, and cannot be entirely replaced, albeit complemented by models.
1 Introduction and aim

Emissions of Organic Chemicals from Technosphere Articles (ChEmiTecs) is a research programme funded by the Swedish Environmental Protection Agency. The programme’s goal is to improve the understanding of emissions of organic substances from articles and to clarify and determine the magnitude of this problem.

This study addresses one of the main objectives of ChEmiTecs, to assess the importance of emissions from articles in relation to other emission sources and pathways. To achieve this, the knowledge gained regarding emissions of selected chemicals from articles has been related to emissions from other sources. More specifically, the following issues have been addressed:

- To assess the importance of diffusive emissions of selected substances in relation to other sources on the national and local, urban scale (Stockholm).
- To develop a systematic assessment method that can be applied also to other chemicals in the future.

1.1 Background

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. Four alternative methods to estimate emissions were included in Cousins (2013):

a) Population-based extrapolation of a national substance flow analysis (SFA) study combined with technical information for homologue specific release estimates
b) Region-specific SFA calculations
c) Inverse multimedia fate modelling
d) Experimental measurements of source-specific release rates

Strengths and weaknesses of each of these methods were discussed and it was concluded that the methods are complementary and that cross-checking by using a combination of different methods is preferable. Within ChEmiTecs, the three methods b), c) and d) have been applied to estimate emissions from articles and from other sources (Westerdahl et al., 2012; Cousins, 2013; Holmgren, 2013). In addition, a fifth method (e), represented by the use of a mechanistic emission model (Holmgren et al., 2012) can be added to this list.

To study emissions from articles in a comprehensive manner, the ChEmiTecs programme has focussed on a number of case study articles, which exist in large quantities and have a use pattern which can give rise to emissions of organic chemicals. For each article, a specific substance of concern was selected (Table 1). The selection process has been described in detail by Andersson and Rännar (2009) and Rännar and Andersson (2010). The first five case studies were selected at the beginning of the project, while a sixth case study (diuron in indoor paint), was added at the end of the project, when detailed data regarding chemical composition of indoor paint were made available.
Table 1 Case study articles and their corresponding chemicals

<table>
<thead>
<tr>
<th>Article</th>
<th>Substance</th>
<th>CAS-numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. PVC flooring</td>
<td>Diisononylphthalate (DINP)</td>
<td>28553-12-0</td>
</tr>
<tr>
<td>2. LCD screens</td>
<td>Triphenyl phosphate (TPP)</td>
<td>115-86-6</td>
</tr>
<tr>
<td>3. Concrete foundations</td>
<td>Tributyl phosphate (TBP)</td>
<td>126-73-8</td>
</tr>
<tr>
<td>4. Tires</td>
<td>Benzothiazole-2-thiole (MBT)</td>
<td>149-30-4</td>
</tr>
<tr>
<td>5. Jackets</td>
<td>8:2 fluorotelomer alcohol (8:2 FTOH)</td>
<td>678-39-7</td>
</tr>
<tr>
<td>6. Indoor paint</td>
<td>Diuron</td>
<td>330-54-1</td>
</tr>
</tbody>
</table>

Emission measurements and detailed literature studies for the case study objects provided the basis for the development of a generic, predictive emission model, the purpose of which is to perform quantitative calculations of emissions of chemicals from materials in consumer products during their service life. This work has been described in a doctoral thesis published by Holmgren (2013).

To estimate nationwide emissions of case study substances and other organic chemicals, the accumulated stock of selected products was described, taking into account the surface area, the material composition of the products and the chemical composition of the materials; see Westerdahl et al. (2010) for a description of the methodology. This information was then used as input to the generic emission model described in Holmgren (2013). Nationwide emissions of organic chemicals from selected consumer products in the Swedish society, among them the case study articles, have also been estimated (Holmgren and Haglund, unpublished data) and have been applied in the current report.

Information regarding important complementary emission sources has been compiled for the case study substances using SFA methodology. In the SFAs the most important emission sources and pathways for the selected chemicals have been identified using both emission estimates for different emission categories as well as environmental data. The SFA methodology and the results from the first five case studies are given in Westerdahl et al. (2012). The SFA for diuron is presented in Lexén et al. (2014).

Environmental fate models are useful tools to cross-check emission estimates as pointed out in Cousins (2013). These can create a link between estimated emissions and observed environmental occurrence and help to understand if the current knowledge about chemical emissions and transport pathways can explain the occurrence in the environment (Figure 1). They can also be applied according to method c) above, to back-calculate emissions from environmental monitoring data. For example, Moeckel et al. (2010) used a modelling approach to back-calculate emissions of PBDEs in the urban area of Zürich, Switzerland, based on observed atmospheric diel patterns.
Assessing the relative importance of emissions from articles of selected organic substances

When multimedia fate models are applied, the environmental system under study has to be defined. In essence, this means setting the 3-dimensional boundaries for the geographical region of interest. The ChEmiTecs case study objects cover a variety of article-chemical combinations which are typically used either indoors (TPP in flat screen displays) or outdoors (TBP in concrete, MBT in car tires), but some of them have multiple uses, such as DINP in PVC which occurs both in indoor and outdoor applications. To assess the emissions from such a variety of products a multimedia tool was required which could take into account emissions indoors and outdoors as well as the interactions between the two environments. Because of the high density of consumer products as well as humans, urban areas are of special interest for assessing the importance of emissions from consumer products.

Previously developed urban modelling tools (Diamond et al., 2001; Palm, 2001; Prevedouros et al., 2008) have not considered the indoor environment as an integrated part of the urban system. Similarly, existing indoor models have not been included in an urban context (Bennett and Furtaw, 2004; Zhang et al., 2009). This was considered a weakness for the purpose of the ChEmiTecs research programme, leading to the development of the Stockholm Multimedia URban Fate (SMURF) model (Cousins, 2012).

Figure 1. Schematic overview of the connection between emissions and environmental occurrence, and how different assessment methodologies apply in different steps.
Assessing the relative importance of emissions from articles of selected organic substances

2 Methods

To assess the relative importance of emissions from articles compared to emissions from other sources, two different approaches have been used:

i. Estimates of nationwide emissions from consumer articles were compared to emissions from other sources and pathways obtained from the SFA studies, such as industry and/or atmospheric deposition.

ii. 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. Model predicted environmental concentrations were compared to monitoring data to find out if emissions from articles and M-WWTPs may explain the concentrations found in the environment.

2.1 Comparing emissions from articles with estimated emissions from other sources

Within the ChEmiTecs programme, emissions from consumer articles (Cousins, 2013; Einarson, 2009; Holmgren, 2013; Molander et al., 2012; Westerdahl and Rydberg, 2011) as well as from other sources (Westerdahl et al., 2012) have been estimated. To assess the importance of emissions from consumer articles, the emissions from consumer articles were compared with emissions from other sources, such as industry.

Emissions from articles were studied through experimental studies (Cousins et al., 2013; Holmgren et al., 2013a; Holmgren et al., 2013b) and comprehensive literature studies (Einarson, 2009). Together, these formed the basis for the development of a generic emission model (Holmgren et al., 2012). The model was used to calculate emissions to air, indoor air and wastewater of a wide range of substances and articles (Holmgren and Haglund, unpublished data). The estimated emissions are presented in Table B1 in Appendix B.

In Westerdahl et al. (2012), SFA methodology was applied to estimate releases of the case study chemicals from sources other than consumer articles, which contribute to the environmental burden of organic chemicals. Data from these studies consist of information and estimations of the industrial use of each case study substance within Sweden, import of the substance, emissions from industry, municipal wastewater treatment plants and landfills as well as data on atmospheric deposition.

In this report, we summarize the findings from Westerdahl et al. (2012) and compare them to the estimated emissions from articles described above, to assess the magnitude of the emissions from products relative to other sources. In this perspective it was important to distinguish between a source and a transport pathway. Industrial releases (to air, water, soil and wastewater) are considered to be sources, whereas release from M-WWTPs and atmospheric deposition are considered to be transport pathways. The estimated annual load via different sources and pathways are also compared to the import of the substance within products. Based on these comparisons, the impact of emissions from articles is assessed.
Assessing the relative importance of emissions from articles of selected organic substances

2.2 Evaluating the importance of emissions from articles using the SMURF model

2.2.1 The SMURF model

The SMURF model has been described in detail in Cousins (2012). It is a local-scale, eight-compartment, fugacity-based, non-equilibrium, steady state multimedia fate model parameterized to the municipality of Stockholm. It includes air, surface water, soil, sediment, urban film, indoor air; indoor horizontal surface and indoor vertical surfaces including ceilings. The model addresses intermedia transfer as well as degradation and advective removal from the different compartments (Figure 2).

![Diagram of SMURF model](image)

**Figure 2.** Illustration of the compartments and dimensions in the SMURF model and the processes considered.

2.2.2 Model input

In addition to geophysical characterization of the model environment, as given in Cousins (2012), the model requires input data on physical-chemical properties, background concentrations in air and/or water and emissions. Property data and background concentrations used are given in Table B 2 and Table B 3 in Appendix B.

Emissions used are presented in Table B 1 in Appendix B. National emissions from articles, estimated as described in 2.1, were scaled to the municipality of Stockholm based on population through multiplication by the Stockholm/Sweden population ratio 0.09. Emissions to surface water and soil were taken from Westerdahl et al. (2012) – see Table B 1 in Appendix B. These are further discussed in chapter 0.

Since the SMURF model treats input parameter uncertainties by applying 95% confidence factors (CFs), the emission ranges were expressed in this way, through the application of CFs. With this approach, all input parameters are assumed to have a log-normal distribution. A CF of 5 implies that with 95% certainty, the true value of an input parameter assigned a value of X lies within the range X/5 – X×5. A CF of 5 was applied to all emission estimates, generating the ranges presented within brackets in Table B 1. For releases to surface water and soil sometimes no median value was given (see Appendix 0). In this case a mid-point value of the given range was adopted, and ranges re-calculated using the confidence factor.
2.2.3 Model simulations

The SMURF model was run for the six substances specified above. Model predicted concentrations in indoor air, indoor dust, outdoor air, surface water, sediments and soil were compared to monitoring data (Monitoring data used for model evaluation).

For TPP and TBP, concentrations in fish were used to estimate surface water concentrations. Measured concentrations in perch in lakes near Stockholm were determined to 32-150 ng/g lw for TPP and to 14 - 4900 ng/g lw for TBP (Sundkvist and Haglund, 2009). Using a fat content of 0.5 % and a BCF of 74 and 69.6 L/kg ww for TPP and TBP, respectively (calculated using the Arnot-Gobas method, EPIWEB software, USEPA (2011)), the corresponding water concentrations were calculated to be 2-10 ng/L and 1-350 ng/L for TPP and TBP, respectively.

Table B 3 in Appendix B), to assess whether the assigned emissions from articles may explain the concentrations found in the environment. Emissions released via M-WWTPs were also included, arguing that a large proportion of these, albeit not all, are derived from households and consumer goods. Possible reasons for discrepancies were discussed, and in some cases inverse modelling was applied to highlight the likely size of emissions needed to explain the observed concentrations. The underlying principle behind the approach is illustrated in Figure 3.

![Figure 3. Methodology to evaluate the importance of emissions from consumer articles on the occurrence of organic chemicals in the urban environment, using the Stockholm Multimedia Fate Model](image-url)
3 Results and discussion

The overall findings from the emission assessments are summarized in Table 2, and the conclusions derived using the two assessment methods are compared. In the subsequent chapters, the results are presented in more detail. The results from the SFA methodology are presented in chapter 3.1 and results based on application of the SMURF model are presented in chapter 3.2.

Table 2. Summary of the major findings related to the importance of emissions from articles using two different approaches.

<table>
<thead>
<tr>
<th></th>
<th>SFA assessment Sweden</th>
<th>SMURF model assessment Stockholm</th>
</tr>
</thead>
<tbody>
<tr>
<td>DINP</td>
<td>The SFA method suggests that industrial emissions override estimated emissions from consumer articles and that industry is an important contributor to DINP in M-WWTP influents. Release via contaminated sludge is identified as a major transport pathway to the environment and atmospheric deposition should also be considered. In later years (2013), DINP has been replaced by other substances, and the importance of industrial releases is likely to be decreasing.</td>
<td>Emissions from products and M-WWTPs to indoor and outdoor air and surface water explain concentrations found in the indoor environment, but not in the outdoor urban environment. 200 and 800000 times higher emissions/background inflow to outdoor air and surface water are required to explain the levels in air and sediments. This implies that industrial or additional product derived emissions are needed to explain levels found in the outdoor environment. Lack of monitoring data in soil, surface water and inflowing air cause uncertainties in the results.</td>
</tr>
<tr>
<td>TPP</td>
<td>Industrial emissions are more important for the release of TPP than those of the articles included in the case study, but it was highlighted that many articles were missing in the assessment. In addition, a large proportion of the identified industry emissions are in fact directed to incineration and it was concluded that emissions from articles may be in the same order of magnitude as industrial emissions.</td>
<td>Current emissions from products to Stockholm indoor air are in the range 1.0 kg/year or 1.2×10⁴ kg per capita and year and these explain concentrations found in the indoor environment. Concentrations in the aquatic environment are explained by the high estimated background atmospheric inflow of 10 tonnes/year (12 ng/m³), but due to the lack of monitoring data for many other matrices firm conclusions could not be drawn.</td>
</tr>
<tr>
<td>TBP</td>
<td>Missing information on emissions from industry and only rough estimates on releases from articles hinders a comparison between the two categories. Leakage from hydraulic fluids, atmospheric deposition and release via M-WWTP effluents are potentially important transport pathways.</td>
<td>TBP emissions from products are severely underestimated. Using backwards modelling resulted in indoor air emissions of 3.4×10⁵ kg per capita and year, the majority of which will reach the outdoor air compartment. These emissions will still underestimate dust levels, implying that abrasion and/or direct migration to dust may be important. Atmospheric inflow concentrations of 150 ng/m³ are required to explain the measured deposition rates. The highest estimate for emissions to indoor air results in outdoor air concentrations of similar order of magnitude as measured concentrations at background stations. These findings suggest that the contributions of the indoor environment to outdoor air may be significant.</td>
</tr>
</tbody>
</table>
Assessing the relative importance of emissions from articles of selected organic substances

<table>
<thead>
<tr>
<th>MBT</th>
<th>Information on industrial emissions of MBT was not obtained. Releases via M-WWTPs are assumed to be the most important pathway to the environment, to which both industry and households are likely to contribute. Release from abraded tyre particles may be an important release pathway.</th>
<th>The available urban monitoring data did not allow a reliable comparison, but current emission estimates result in possible underestimated concentrations in the aquatic environment. This indicates that emissions to water are potentially larger than current estimates. Emissions to air could not be evaluated (all measured concentrations were below the detection limit), but resulted in a slight overestimation of atmospheric deposition compared to measurements.</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.2 FTOH</td>
<td>Insufficient information for proper assessment. Information from other countries indicates that emissions from articles are important.</td>
<td>Applying per capita emissions calculated for Zürich of 5.97×10⁻⁶ kg per capita and year and a background concentration of 0.014 ng/m³ resulted in predicted concentrations in indoor air and air similar to measured concentrations in Norway and Canada, but an underestimation of dust levels. Due to the lack of Swedish monitoring data the emission estimates could not be properly evaluated.</td>
</tr>
<tr>
<td>Diuron</td>
<td>Emissions of diuron from painted walls and during painting were estimated to 61 kg/year, of which the majority is directed to wastewater. The import as a pure substance exceeds 10 tonnes per year, thus industrial emissions during manufacture are expected.</td>
<td>Emissions to indoor air and surface water from painted walls and M-WWTPs and background inflow resulted in underestimation of outdoor environmental concentrations, implying that the estimated emissions from articles do not explain the concentrations found in the environment.</td>
</tr>
</tbody>
</table>

### 3.1 Comparing emissions from articles with estimated emissions from other sources

#### 3.1.1 Diisononylphthalate (DINP)

The main application of diisononylphthalate (DINP) is as a plasticizer in flexible PVC, which is used in articles such as flooring, industrial hoses and tubing, toys and food contact plastics (SPIN, 2014). Examples of non-PVC applications are in rubbers, adhesives, sealants, paints, lacquers and lubricants (ECB, 2003).

The import of DINP as a pure substance for use within the Swedish industry was approximately 12 000 tonnes in 2009 (SPIN, 2014). No data have been found on import of DINP in finished articles. Less than 0.1% of the DINP used within industry, approximately 16 tonnes, is emitted yearly during industrial processing of PVC (ECB, 2003). Half of this is emitted to M-WWTPs and half to air.

It is worth noting, that in later years (2013), the use of DINP has decreased substantially and is now being replaced mainly by diisononyl cyclohexane-1,2-dicarboxylate (DINCH), thus the industrial releases of DINP are likely to have decreased since 2009.

Annual emissions to Swedish indoor air from PVC flooring were estimated to be 40 kg ± 18 kg (Holmgren et al., 2012). Emissions to indoor and outdoor air and wastewater from other products such as electronic equipment, foam mattresses and rain jackets were estimated to be about 0.3 kg/year (Holmgren and Haglund, unpublished data), i.e. insignificant compared to the estimated releases from flooring. The total estimated
emissions from products are thus significantly lower than the industrial emissions. However, several products are missing from this assessment, e.g. PVC wall covers, outdoor roofs etc., thus the true emissions from consumer articles are likely to be higher. Yet, considering the large discrepancy between the estimated emissions from industry and products (factor of 400) it is unlikely that these additional consumer-related emissions would exceed the estimated industrial emissions.

Looking at the pathways, transport via M-WWTPs appears to be a major release route for DINP from the technosphere. The releases mainly occur via different applications of contaminated sludge, and industry is likely to be one of the main sources. The fate of DINP released to soil via contaminated sludge is treated in chapter 3.2.1. Atmospheric transport followed by atmospheric deposition is also a possible pathway, but the magnitude of the atmospheric deposition is very uncertain, considering the limited availability of deposition data for DINP. The estimate presented in Figure 4 is based on one single measurement in Denmark.

![Figure 4. Import, emissions and flows of DINP in the Swedish society. Note that emissions from consumer articles do not cover all DINP containing products, thus emissions from all consumer products are likely to be higher. Atmospheric deposition is denoted with a striped bar, since this estimate is considered to be more uncertain than the others.](image)

### 3.1.2 Triphenyl phosphate (TPP)

Triphenyl phosphate (TPP) can be used for a wide variety of applications, for example as flame retardant or as plasticizer. Approximately 50 % of the TPP is used as a flame retardant in PVC, where it also serves as a plasticizer (OECD, 2002). TPP is also used as a flame retardant in other polymers, in printed circuit boards and in photographic films as well as in applications such as hydraulic fluids, adhesives, inks and coatings (OECD, 2002).

The import of TPP as a pure substance for use within the Swedish industry was approximately 70 tonnes in 2009 (SPIN, 2014), where the majority was used as raw materials in the production of plastics. Industrial emissions have been estimated to 1 100 kg/year, where the two main recipients are water, 400 kg, and waste, 600 kg. The solid
waste is expected to be subject to incineration, whereby most of the TPP is expected to degrade or be transformed.

Import of TPP in flat panel displays has been estimated to 30 000 kg/year (Westerdahl et al., 2012). Emissions from use of consumer articles have been estimated for flat panel displays to 3.9 kg/year (Holmgren et al., 2013b) and upholstered furniture such as sofas, mattresses and office chairs, 7.6 kg/year (Holmgren and Haglund, unpublished data). Altogether this results in emissions from consumer articles amounting to 11.5 kg/year (see Table B 1 in Appendix B), i.e. a factor of 100 lower that the estimated releases from industry in the form of release to waste and wastewater. These consumer articles only constitute a fraction of the TPP-containing consumer articles, thus the true emissions of TPP from all consumer product are likely to be higher. Taking into account that a large proportion of the industry related emissions were directed to incineration, it is possible that the actual emissions from products are in the same order of magnitude as those from industry.

The release via M-WWTPs occurs through transport via WWTP effluents (100 kg/year) and via application of sludge (80 kg/year). In total the releases via M-WWTPs are estimated to be 180 kg/year. Approximately 20 kg is estimated to be transported to landfills, from where it may be further released to the environment through landfill leachate. Release via landfills is estimated to be 44 kg/year.

Air transport and atmospheric deposition are possible pathways for the transport of TPP; however, the magnitude of the atmospheric deposition is very uncertain as the estimate is based on a single measurement from a remote location in northern Finland.

<table>
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<th>Pure subs.</th>
<th>Flat panel displays</th>
<th>Industry</th>
<th>Flat panel displays</th>
<th>Upholstered furniture etc.</th>
<th>Atm. dep.</th>
<th>M-WWTP</th>
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Figure 5. Import, emissions and flows of TPP in the Swedish society. Note that emissions from consumer articles do not cover all TPP containing products, thus emissions from all consumer products are likely to be higher.
3.1.3 Tributyl phosphate (TBP)

The main use of tributyl phosphate (TBP) is as a flame retardant in aircraft hydraulic fluid and as a solvent for rare earth extraction and purification (OECD, 2002). More than 80 \% of the TBP is used for these applications. Minor uses of TBP are as a defoamer in cement casings for oil wells, as a flame retardant in polymers or as an anti-air entrainment additive for coatings and floor coverings.

The Swedish industry imported approximately 30 000 kg of TBP as a pure substance in 2009 (SPIN, 2014), where the majority was used as anti-foaming agents. No data has been found regarding emissions from industrial use of TBP.

Import of TBP in hydraulic aircraft fluids has roughly been estimated to 100 000 kg/year (Westerdahl et al., 2012). Assuming that 10\% of the hydraulic fluid is released into the environment yields an emission of 10 000 kg/year. It should be noted that this is a very rough estimate. Emissions of the related substance triisobutylphosphate (TiBP) from the concrete foundations of a single bridge have been estimated by (Holmgren et al., 2013a), where the estimate total release was 8 kg emitted over eight years. Because of the structural similarities of the two, we have assumed that TBP emissions from the same bridge would be in the same order of magnitude. As there are no data on emissions from industry, and only rough estimates of emissions from consumer articles, it is difficult to comment on the importance of emissions of TBP from consumer articles in relation to other emission sources.

Air transport and atmospheric deposition are possible pathways for the transport of TBP; however, the magnitude of the atmospheric deposition is very uncertain as the estimate is based on a single measurement from a remote location in northern Finland.

![Figure 6. Import, emissions and flows of TBP in the Swedish society. Emissions from products are mainly represented by releases from hydraulic fluids and a single concrete bridge foundation which are both subject to large uncertainties. Emissions from all consumer products are likely to be higher.](image-url)
3.1.4 Benzothiazole-2-thiole (MBT)

Benzothiazole-2-thiole (MBT) is a High Production Volume (HPV) chemical, with production in six EU countries. There is no production of MBT in Sweden. The main use is in the rubber industry as a non-volatile vulcanisation accelerator but also as an intermediate in the production of other accelerators, some of which may decompose during vulcanisation and form MBT. Approximately 4 tonnes MBT is annually imported to Sweden as pure substance. The imported amounts of MBT in products are unknown.

In a recent Swedish screening study of benzothiazoles (Brorström-Lundén et al., 2011) MBT showed high detection frequencies in biota samples such as mussels (81 %) and fish (75 %), and was also found in some surface water samples (detection frequency of 36 %). It was also commonly found in samples related to release pathways, i.e. storm water, landfill leachate, M-WWTP effluents and M-WWTP sludge. However, MBT was not detected in air or deposition and also not in crops, soil or sediments. The occurrence in M-WWTP samples indicates that release via M-WWTPs is an important pathway of MBT to the aquatic environment where it accumulates in biota. The occurrence of MBT in storm water indicated that traffic related emissions will take place. Air transport seemed to be of minor importance.

The emissions of MBT from consumer articles to indoor and outdoor air were estimated to 94 kg by Holmgren and Haglund (unpublished data), using the emission model developed by Holmgren et al. (2012). The majority of this amount was attributed to releases from tyres in storage and by diffusion from abraded particles. Quantitative information on releases from industry to wastewater has not been obtained. It is anticipated that industrial sources together with households contribute to the inflowing amounts to the M-WWTPs, from where approximately 400 kg MBT may annually enter the environment via effluent water. Another 40 kg may be released via application of contaminated sludge in various contexts. Some release via landfill leachate is also possible.

![Figure 7. Import, emissions and flows of MBT in the Swedish society.](image-url)
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3.1.5 8:2 Fluorotelomer alcohol (8:2 FTOH)

No data were found on the Swedish use of 8:2 FTOH. Internationally, FTOH is manufactured as a raw material used in the synthesis of fluorotelomer-based surfactants and polymeric products, and may be present as an undesired, un-reacted residual in the final product by up to 0.1-0.5 wt % (Prevedouros et al., 2006). The manufacture of FTOHs usually results in a mixture containing six to twelve fluorinated carbon congeners with the 8:2 FTOH being the dominant one. In 2006, there were four manufacturers of fluorotelomer-based raw materials in three different countries (USA, Germany and Japan). The global production of FTOH was estimated to approximately 11000-14000 tonnes/year.

The fluorotelomer alcohols are used to treat paper to improve its moisture and oil barrier properties. FTOHs are also used in waterproof outdoor clothing and in waterproofing agents for textiles. 8:2 FTOH have been detected in several consumer products, such as, textile- and leather furniture, shoes, ink, carpets, paper and outdoor clothing (see Westerdahl et al. (2012) and references therein). Unreacted telomer alcohols can potentially gas-off both during production of the monomer and from polymeric materials that contain FTOH.

Due to its characteristic surface-active properties, the model developed by Holmgren et al. (2012) proved not to be suitable for predicting emissions from consumer articles of 8:2 FTOH. The estimated emissions from articles were thus considered to be severely underestimated. Only emissions from surface treated jackets were calculated, and these were estimated to 0.06 kg/year. For comparison, indirect releases from the indoor environment were estimated to be 60 kg/year, based on indoor air concentrations in Norway (Westerdahl et al., 2012). Swedish monitoring data for indoor air are lacking, however. Similarly, Norwegian data on M-WWTP sludge and effluent water indicate environmental releases to surface water and soil of about 10 kg/year (Westerdahl et al., 2012).
3.1.6 Diuron

Diuron is a high production volume chemical which is mainly used as a herbicide but may also be used as active substance for film preservatives and masonry preservatives. Since 2008, diuron is no longer approved in antifouling products (product group 21) and since 2009, use of diuron as an active substance in in-can preservatives (product group 6) is neither approved in the EU.

In Sweden, diuron has been used as an active substance in a total of 18 herbicide preparations until the year 1992. Today, there are no new approved herbicidal preparations containing diuron in use in Sweden (KEMI, 2013).

There has been more than a twentyfold increase in the number of diuron-containing preparations since the early 90’s, from six preparations in 1992 to 129 preparations in 2011 and the total use of diuron in chemical preparations in Sweden was approximately 20 tonnes in 2011. During the time period 1999-2011, the use of diuron has fluctuated between 4 and 58 tonnes per year, with the highest value 2008, import in finished articles excluded. Thus the true import could even be higher.

The emissions during service life of paint for inner walls have been estimated, both during painting and from dry paint. Approximately 60 kg diuron was estimated to be emitted to waste water during painting while approximately 1 kg is estimated to be emitted to indoor air from dry paint each year (Molander et al., 2012). It should be noted that the emission estimate to waste water is a rough estimate. The major known release pathway of diuron to the environment is via the M-WWTPs.
3.2 Evaluating the importance of emissions from articles using the SMURF model

The results from the modelling exercises using the SMURF model are presented and discussed per substance in chapters 3.2.1 to 3.2.6. Monitoring data used for comparison were taken from Westerdahl et al. (2012), and from references therein, or otherwise specified. Mainly data from Stockholm have been included, but in some cases also data from other locations have been included, the relevance of which is discussed in the context of the substance.

3.2.1 Diisononylphthalate (DINP)

Figure 8 shows a comparison of model predicted and measured concentrations of DINP. The figure also shows the predicted steady state environmental distribution of the substance, as well as the steady state mass and residence time of DINP in the Stockholm environmental system, as a result of the estimated product-related emissions including release via M-WWTPs, and the background atmospheric inflow. Because of the large estimated releases to urban soil via contaminated sludge, the vast majority of DINP is predicted to reside in soil but the chemical will also partition to indoor surfaces and urban sediments at steady state. The predicted steady state mass is 110 kg with a residence time of 1600 hours. This refers to the “free” substance, i.e. not chemical incorporated in products, and represents about 19 % of the estimated annual release (emissions+ background inflow). The relatively slow turnover of DINP in the Stockholm environment is a result of the high estimated releases to soil, where soil reaction is the dominant removal pathway. This is a relatively slow process compared to e.g. advection in air, which rapidly removes chemical from the air compartments to surrounding areas. This is discussed further in section Error! Reference source not found. (Figure 16).

The results indicate that the indoor emissions (3.6 kg/year in Stockholm or 4.1×10^6 kg per capita and year) can explain the concentrations found in indoor air and dust, i.e. the emissions to indoor air appear to be in the right order of magnitude, with an agreement between modelled and measured concentrations of a factor of 1-3. However, outdoor air concentrations are underestimated by about a factor of 40 and also urban sediment concentrations are severely underestimated (factor of 900).

![Figure 8](image_url)
Potential explanations to the disagreement between modelled and measured outdoor levels are:

i) Underestimation of the background inflow with air (0.25 ng/m$^3$ or 210 kg/year). The applied value represents the detection limit and the median value from samples taken on the Swedish west coast in a previous environmental screening study ($n=3$, Cousins et al. (2007)). Apart from the uncertainty associated with the few number of samples, inflowing air to Stockholm is not unaffected by anthropogenic activities, thus it may be erroneous to adopt remote concentrations to represent regional background concentrations. A targeted downwind semi-urban – urban monitoring campaign would be helpful to address this issue.

ii) Missing product-related sources in the outdoor environment. Despite the efforts within ChEmiTecs to calculate emissions of case study substances from all consumer articles, this was not possible for a variety of reasons. Also, the emission model does not take into account abrasion of materials that could potentially lead to release of DINP-containing particles which may be transported to the outdoor environment e.g. via sewage systems. Kaj et al. (2010) measured DINP concentrations in wastewater effluents, which were all below the detection limit, generating an estimated annual release range of 0–0.5 tonnes in Sweden or 0 – 45 kg in Stockholm, based on the detection limits (Westerdahl et al., 2012). Applying the higher value (45 kg/year) would generate sediment concentrations of 9.6 ng/g dw which is still a factor of 200 lower than the measured concentrations. It seems unlikely that the missing emissions are derived from the indoor environment, considering the good agreement with monitoring data for indoor air and dust, and the low predicted outflow from indoor surfaces (0.75 kg/year). Run-off from urban surfaces (1 kg/year) could be higher if the background atmospheric inflow is underestimated. There may however be other products, particularly products used in outdoor applications that could generate emissions to outdoor air and surface water, most likely canalised via the storm water system. In the EU risk assessment for DEHP, “waste remaining in the environment” was identified to be a large potential source and carrier of phthalates. It is possible that such waste, i.e. abraded particles and fragment of rubbers and plastics, which enter the aquatic system, is part of the explanation of the higher levels in sediments compared to the model predictions. To explain the levels found in the outdoor environment (air and sediments) emissions to outdoor air and to surface water (alternatively background inflow) had to be increased to 5 and 10 tonnes per year, respectively. This is 200 times higher than estimated maximum emissions to water based on M-WWTP effluents, and regarding air, 5 tonnes per year (or a background concentration of ca 6 ng/m$^3$) would result in a net transfer of DINP from the outdoor to the indoor environment. The prevailing data set on outdoor levels is still limited, leaving uncertainties in the assessment. In particular, concentrations in soil, surface water and inflowing air (urban background) are still lacking.

iii) Locally affected sampling sites. There is a possibility that the samples collected in outdoor urban air and sediments may be affected by local sources near the sampling point, and therefore not reflect the “average urban situation” as predicted by the model. As mentioned previously, additional
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...semi-urban air monitoring, away from the close proximity of i.e. buildings, as well as a larger coverage of sediment samples would provide useful information to further explore this issue.

3.2.2 Triphenyl phosphate (TPP)

Figure 9 shows the predicted and measured concentrations of TPP, as well as the predicted steady state mass, residence time and environmental distribution, based on estimated product-related emissions. As shown in the figure, no data were found on urban outdoor air, soils, sediments or surface water. The majority of TPP is predicted to reside in soil, urban sediments, urban film and surface water and amounts to ca 370 kg with a residence time of 319 hours. This represents about 3.6% of the estimated annual release (emissions+ background inflow). The majority of these amounts are attributable to the estimated background inflow with air.

The results indicate that the indoor emissions (1.0 kg/year in Stockholm or 1.2×10^6 kg per capita and year) and the background inflow of 10 tonnes/year (12 ng/m^3) can explain the concentrations found in indoor air and dust, as well as in surface water as estimated from measured concentrations in fish (Appendix 0), implying that the emissions and background inflow appear to be in the right order of magnitude, with an agreement between modelled and measured concentrations of a factor of 1-5. However, due to the lack of monitoring data in many of the outdoor matrices it is still early to draw firm conclusions.

![Figure 9. Comparison of model predicted and measured concentrations of TPP using the SMURF model. Model predictions are based on ChEmiTecs estimated emissions from articles and M-WWTPs and a background concentration of 12 ng/m^3.](image-url)
3.2.3 Tributyl phosphate (TBP)

Figure 10 shows the predicted and measured concentrations of TBP, as well as the predicted steady state mass, residence time and environmental distribution, based on estimated product-related emissions. As shown in the figure, the monitoring data availability is scarce. The majority of TBP is predicted to reside in surface water and urban sediments and with small proportions in soil and outdoor air, with a total estimated steady state amount of 7.3 kg and a residence time of 123 hours. This residence time is fairly short relative to the large amounts released, due to rapid degradation in water and air, but also to the fast advective removal with air and water (see Figure 16). The predicted steady state amount represents about 1.4% of the estimated annual release (emissions + background inflow). The majority of these amounts are attributable to the estimated emissions to surface water.

As evident from the figure, the estimated emissions result in predicted environmental concentrations that are a factor of 13-70000 times lower than measured median concentrations, with worst agreement for indoor air and dust. Emissions to indoor air thus appear to be severely underestimated. The model predicted air-surface deposition (neglecting diffusion) is about 0.03 kg/year. This can be compared to the estimated atmospheric deposition based on measured deposition rates of 230 ng/m$^2$ day which would correspond to 18.5 kg/year Stockholm, i.e. a factor of 600 higher than the model predicted deposition rates, indicating that outdoor air levels may be severely underestimated. Without urban air monitoring data it is not possible to fully evaluate the accuracy of these predictions.

One additional source which is not considered in the current assessment is leakage from hydraulic oils where TBP is used as a flame retardant. The SFA indicates that this usage may result in releases of up to 10 tonnes per year, but the recipient of these emissions is unknown and could therefore not be simulated.

To achieve agreement between predicted and measured concentrations in indoor air and to further improve the agreement for surface water, a backwards modelling approach was applied. Emissions to indoor air and surface water were assigned so that the model predicted concentrations in indoor air, floor dust and surface water agreed with the monitoring data by Haglund and Marklund (2005), Bergh et al. (2011b) and Sundkvist and Haglund (2009), see Table B 3. This resulted in annual emissions of 30 (6 – 150) kg (3.4×10$^{-5}$ kg/capita) to indoor air and 1000 kg to surface water. With these emission estimates, the agreement obtained between predicted and measured concentrations in indoor air, surface water and floor dust was within a factor of 1, 4 and 200 respectively,
and the predicted concentrations all lie within the measured ranges (Figure 11), implying that emissions to indoor air and surface water in Stockholm lie within this range. The remaining relatively large discrepancy between modelled and measured median concentration in floor dust, may be an indication of additional indoor emission pathways such as abrasion or direct migration into dust rather than emissions to indoor air and subsequent deposition to dust. Model predicted atmospheric deposition increased slightly to 0.04 kg/year with these new emission figures, which is still a factor of 460 lower than measured deposition rates. Inflowing air concentrations of 150 ng/m$^3$ would be required to match the measured deposition rate. The majority of the chemical released to indoor air will be transported with the ventilation system to outdoor air. Based on this alternative scenario, emissions to indoor air would result in an annual outflow to outdoor air of 29 kg in Stockholm.

Upscaling the indoor emissions to the whole of Sweden based on population results in national emissions of 330 (67 – 1700) kg to indoor air with an outflow of 320 kg/year to outdoor air. The emissions to surface water are estimated to be 11 000 (2200-55000) kg/year. Emissions to water should be regarded as indicative only, since data for the aquatic environment are still largely missing, but the estimated range covers the estimated releases to water via M-WWTPs of 3000 (30-10000) kg/year in Sweden, (see section 3.1.3) which would represent 270 kg/year in Stockholm, scaled based on population.

Figure 11. Alternative scenario for TBP, obtained using backwards modelling.

TBP has a relatively quick turnover in air, and will be degraded in indoor as well as in outdoor air (Figure 16), but a substantial amount will be transported out of the urban system, leaving only a small percentage in air at steady state, compared to the predicted amounts residing in the aquatic environment. Partitioning to indoor surfaces is predicted to be insignificant (Figure 10), but considering the underestimation of measured dust levels, abrasion and direct migration to dust may be important processes currently not captured in the assessment.
3.2.4 Benzothiazole-2-thiole (MBT)

Figure 12 shows the predicted and measured concentrations of MBT, as well as the predicted steady state mass, residence time and environmental distribution, based on estimated product-related emissions. As shown in the figure, no data for the indoor environment were obtained, and the majority of the measured concentrations were below the detection limits.

MBT is predicted to predominantly partition to soil, surface water and urban surfaces, with a total estimated steady state amount of 2.0 kg and a residence time of 367 hours. This represents about 4.2% of the estimated annual release (emissions + background inflow). The majority of these amounts are attributable to the estimated emissions to outdoor air. Emissions to tyre storage warehouses etc. were regarded as directed to outdoor air, since the definition of indoor air in the SMURF model is narrower, and it was assumed that MBT released in such locations would eventually reach the outdoor air compartment.

As shown in the figure, the estimated emissions result in predicted environmental concentrations that are a factor of 3-600 lower than the median of the detection limits obtained in measurements. MBT was measured above the detection limit in a few urban sediment samples in levels of 33, 47, and 70 ng/g dw (Remberger et al., 2006) which is at least a factor of 1000 higher than the model predicted concentrations. This indicates that emissions and/or background concentrations are at least not overestimated, and for the aquatic environment possibly underestimated. The model predicted air-surface deposition (neglecting diffusion) is about 8.1 kg/year, which can be compared to the measured atmospheric deposition in Stockholm of <0.4 - 3 kg/year (Westerdahl et al., 2012), i.e. a discrepancy by a factor of 3-20. Interestingly, the model overestimates the deposition rates in this case.

Considering that most of the measured concentrations were below the detection limit, it is difficult to draw conclusions about the importance of product related emissions.
3.2.5 8:2 Fluorotelomer alcohol (8:2 FTOH)

The model predicted and measured concentrations of 8:2 FTOH are shown in Figure 13, as well as the predicted steady state mass, residence time and environmental distribution, based on estimated product-related emissions. Since no Swedish data were found, measured levels were derived from Norway and Canada.

The majority is predicted to partition to soil and sediments at steady state, with an estimated amount of 0.4 kg and a residence time of 295 hours, representing about 3.4% of the estimated annual release (emissions + background inflow). This implies that 8:2 FTOH rapidly leaves the urban system via advective air outflow, due to its high volatility and that the remaining amounts are likely to reside in soil (as a result of direct releases with sludge) where it degrades slowly. However, as evident from the figure, concentrations in air, indoor air and dust are a factor of 8–3.3×10^6 lower than measured levels, implying that indoor emissions are underestimated, or that measured concentrations are not representative for Sweden/Stockholm.

**Figure 13** Comparison of model predicted and measured concentrations of 8:2 FTOH using the SMURF model. Model predictions are based on ChEmiTecs estimated emissions from articles and M-WWTPs and a background concentration of 0.014 ng/m^3

Wang et al. (2012) applied a multimedia model to estimate emissions of 8:2 FTOH and other PFASs in the city of Zurich, based on the observed diurnal pattern in outdoor air. They reported estimated per capita emissions of 5.97×10^{-5} kg/year, which would correspond to 52 kg/year in Stockholm. The authors did not speculate whether these emissions were a result of indoor or outdoor uses, but assigning this value to Stockholm indoor air improves the agreement with monitoring data to a factor of 1–1000, i.e. good agreement for indoor air and air, but still low for indoor dust (Figure 14).

**Figure 14.** Alternative scenario for 8:2 FTOH, obtained using emission rates from Wang et al. (2012).

Because of the absence of 8:2 FTOH monitoring data in Stockholm and Sweden it is not possible to evaluate the preliminary emission estimates, but the findings from Norwegian
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indoor environment suggest higher product-related emissions than those estimated within ChEmiTecs and presented in Table B 1. Another complicating factor is that 8:2 FTOH is known to degrade and form more stable compounds, such as PFOA. Therefore, using monitoring data to back-calculate emissions of 8:2 FTOH can be difficult, in particular for some environmental matrices. The air compartment should be the most suitable matrix for performing such back-calculation exercises.

3.2.6 Diuron

The model predicted and measured concentrations of diuron are shown in Figure 15, as well as the predicted steady state mass, residence time and environmental distribution, based on estimated background atmospheric inflow and product-related emissions to indoor air, surface water and soil via M-WWTPs. No data on indoor levels were found. The estimated background inflow with air (worst-case, based on detection limits) is 0.42 kg/year to compare with the estimated emissions to indoor air of 0.117 kg/year. This atmospheric load results in modelled/ measured agreement for urban surface water, urban sediments and urban soil of within a factor of 20-620. The estimated emissions to indoor air, surface water and soil can thus not explain the concentrations found in the outdoor urban environment.

The majority of diuron is predicted to partition to water and soil at steady state, with an estimated amount of 0.4 kg and a residence time of 608 hours, representing about 6.9 % of the estimated annual release (emissions + background inflow). The majority of these amounts are attributable to the estimated emissions to surface water. This implies that diuron does not bury in sediments but rapidly leaves the urban system via advective water outflow and degradation.

![Figure 15](image)

**Figure 15.** Comparison of model predicted and measured concentrations of diuron using the SMURF model. Model predictions are based on ChEmiTecs estimated emissions from articles and M-WWTPs and a background concentration of 0.5 pg/m³

3.2.7 Stockholm as a source to regional environmental pollution of consumer-related emissions

The predicted overall residence time referred to in sections 3.2.2 to 3.2.6 reflects the time that a substance will remain in the system after cessation of emissions. It does not reveal how the chemical is removed from that system. To judge whether the urban area may act as a source for larger-scale environmental pollution it is necessary to explore the mechanisms by which chemicals are removed from the system. In Figure 16, we present the predicted contribution of different removal pathways to the overall system removal of the substances based on the emission scenarios presented in Table B 1. As highlighted in chapter 3.2, these emission scenarios are not complete, but represent the emissions from M-WWTPs and selected consumer articles.
As the figure shows, advective removal with air and water is predicted to account for 33 – 92 % of the removal for the case study substance in the following increasing order: DINP< MBT<TBP<diuron<TPP<8:2 FTOH. Diuron and MBT are mainly transported with water, whereas 8:2 FTOH, TPP, TBP and DINP are mainly transported with air. The majority of MBT and DINP are expected to be degraded in water and soil, and degradation in water is also predicted to be important for diuron and TBP. This assessment is naturally dependent on the assigned emission scenario, a higher relative release to water will also result in a larger proportion being removed from that compartment, illustrating that the removal pathways are only valid for the emission scenario assessed.

![Figure 16. Predicted contribution of different removal pathways to the overall chemical removal at steady state.](image)

Apart from removal pathways, it is particularly relevant to compare the background inflow to the net outflow in order to judge the potential of the urban area to act as a source. As shown in Figure 17, according to the SMURF model predictions Stockholm may act as a source for release of MBT and diuron, and mainly to the aquatic environment (Figure 16). For the other substances, the advective outflow is similar to or lower than the background inflow with air, thus Stockholm appears to have limited impact on the surrounding environment for these substances. It should be noted that background concentrations in water have been assumed to be zero in this assessment.
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Figure 17. Predicted advective inflow with air compared to predicted outflow with air and water for the case study substances.
4 Uncertainties

This report highlights some of the difficulties in grasping overall emissions from articles and comparing them to other emission sources. SFAs provide a useful first start as they compile the existing knowledge about emissions and synthesise empirical data from the literature. The assessment is, however, highly dependent on high quality input data. Large data gaps of emissions as well as environmental concentrations have been identified, which often makes it difficult to draw firm conclusions. A particular difficulty was associated with obtaining information on chemical content in products. These data gaps generate large uncertainties in emission factors and as a consequence, it is difficult to obtain an overall picture of the flow of a substance in the community and the environment. In addition, there is no built-in evaluation or validation process in the SFA procedure.

Empirical measurements are therefore needed at all stages to a) provide input to emission models and SFA studies, b) to verify predicted deposition fluxes e.g. in the atmosphere and aquatic systems and c) to measure concentrations which can be used for model evaluation and/or validation. Due to time and cost restrictions, it may however not be feasible to perform all necessary measurements. Use of models is therefore crucial.

The value of empirical monitoring data in combination with model assessments has been clearly illustrated in the current assessment. By using monitoring data from the indoor environment in combination with the SMURF model, emissions to indoor air from products used in the indoor environment were estimated to be

- For DINP: $4.1 \times 10^{-6}$ kg/capita and year
- For TPP: $1.2 \times 10^{-6}$ kg/capita and year
- For TBP: $3.4 \times 10^{-5}$ kg/capita and year
- For 8.2 FTOH: $5.97 \times 10^{-5}$ kg/capita and year

where the latter was subject to larger uncertainties, due to the absence of Swedish data. For the remaining substances, monitoring data for indoor air were not available. Using these figures, it was possible to explore the importance of alternative emission pathways such as abrasion or slow, direct migration into dust, in case the emission figure explained the levels in air but not in dust, which was the situation for TBP and 8:2 FTOH. This is interesting, since the current version of the emission model only treats diffusive emissions to air. The potential contribution of the indoor environment to the occurrence of these substances in outdoor air and/or as potential source to wastewater treatment plants was also addressed.

Because of the limitation in the emission model in only treating diffusive emissions to air, potential emissions from articles directly to soil and/or water are neglected. Indirect releases via M-WWTPs were included, but these may per definition also contain chemicals with industrial origin, due to the mixed input to M-WWTPs. As mentioned above, for some cases it was possible to evaluate the potential contribution of chemicals released from the indoor environment to M-WWTP inlets and it was judged to be of minor importance for TBP and DINP. This judgement does not consider washing of textiles, and/or direct release of materials to M-WWTPs, only the estimated contribution as a result of indoor cleaning activities.
Regarding phthalates, Jonsson et al. (2008) estimated the total emissions of the previously used plasticizer diethylhexyl phthalate (DEHP) from PVC floors in Stockholm to 16 tonnes, using 2002 as reference year. This is much higher than our estimated DINP emissions of 3.6 kg/year. The majority of the estimated DEHP emissions were attributed to abrasion, and were based on assumptions of the fraction of floor surfaces and percentage of the floor thickness being abraded etc. Also, the calculations were based on an assumed steady inflow of DEHP in floors, using sales statistics between 1995 and 2000. These were substantially higher than the inflow of DINP-floors which have come into use more recently, and are now already being phased out and replaced by e.g. DINCH (Cousins et al., 2014; Holmgren et al., 2012). It can thus be assumed that abrasion of DINP is substantially lower compared to the DEHP figures reported by (Jonsson et al., 2008).
5 Conclusions and recommendations

The following conclusions are emphasized as a result of the assessment.

✓ Overall, the relative importance of emissions from articles appears to depend on the substance as well as the receiving matrix. 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.

✓ Emissions of chemicals from consumer articles are currently best assessed by combining different estimation methods and should be cross-checked through fitting fate models against empirical monitoring data.

✓ Empirical measurements are needed at all stages in emission assessment, and cannot be entirely replaced, albeit complemented by models.

✓ The indoor environment (air and dust) is suitable for studying, modelling and measuring the emissions from articles.

✓ Per capita emissions to indoor air are estimated to be:
  - For DINP: $4.1 \times 10^{-6}$ kg/capita and year
  - For TPP: $1.2 \times 10^{-6}$ kg/capita and year
  - For TBP: $3.4 \times 10^{-5}$ kg/capita and year
  - For 8.2 FTOH: $5.97 \times 10^{-5}$ kg/capita and year

✓ Additional product-related and/or industrial emissions are needed to explain the concentrations found in the outdoor environment for DINP, diuron and possibly MBT.

✓ Stockholm has limited importance as a regional emission source for DINP, TPP, TBP and 8:2 FTOH, but may be important for MBT and diuron.

✓ Existing data gaps lead to large uncertainties being associated with the results.

For future studies, the following topics are recommended:

✓ Detailed information on chemical composition of materials is urgently needed.

✓ Emission factors for both industrial and product related emissions need to be updated and/or developed.

✓ The role of abrasion and direct migration from products should be addressed in future emission assessments.

✓ To address the background atmospheric inflow, empirical upwind – downwind monitoring studies should be conducted.

✓ Extended environmental monitoring in urban areas (air, sediment, indoor air and dust) is needed to improve our understanding of emissions from articles.
Assessing the relative importance of emissions from articles of selected organic substances

6 References

Andersson P, Rännar S. A report on the initial procedure for identification of chemical/article/use combinations of concern, including the selected case-study chemicals, Umeå, 2009.


Cousins AP, Holmgren T, Remberger M. Emissions of two phthalate esters and BDE 209 to indoor air and their impact on urban air quality. Science of The Total Environment 2013: Accepted.


Cousins AP, Remberger M, Kaj L, Ekshed Y, Dusan B, Brorström-Lundén E. Results from the Swedish National Screening programme 2006 - Subreport 1: Phthalates. IVL Swedish Environmental Research Institute, 2007.


Holmgren T. Emissions of organic compounds from technosphere articles: Measurements and modeling of mass transfer from consumer goods and building materials to air and water. Umeå Universitet, Umeå, 2013, pp. 74.
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Holmgren T, Haglund P. Umeå University, unpublished data.
Sternbeck J, Österäs A-H. Screening of pesticides at golf courses and in urban areas. WSP Environmental, 2010.
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Törneman N, Johansson M. Screening of biocides and organic halogens. SWECO Environment AB; 2009.
Westerdahl J, Hansson K, Cousins AP, Andersson H, Brorström-Lundén E. Emission inventories of different source categories. IVL Swedish Environmental Research Institute, Göteborg, 2012.
Appendix A: Results from the SFAs

Table A 1. Estimated emissions of DINP from different source categories

<table>
<thead>
<tr>
<th>Source</th>
<th>Name flow</th>
<th>Size flow (kg/year)</th>
<th>Released to</th>
</tr>
</thead>
<tbody>
<tr>
<td>Industry</td>
<td>Influent wastewater</td>
<td>8000</td>
<td>M-WWTP</td>
</tr>
<tr>
<td>Industry</td>
<td>Emission to air</td>
<td>8000</td>
<td>Outdoor air</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Effluent wastewater</td>
<td>0-500</td>
<td>Surface water</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sewage sludge</td>
<td>4000</td>
<td>Soil</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sewage sludge</td>
<td>2000</td>
<td>Waste disposal (incineration and landfills)</td>
</tr>
<tr>
<td>Landfills</td>
<td>Leachate</td>
<td>0.5</td>
<td>Surface water</td>
</tr>
<tr>
<td>Landfills</td>
<td>Leachate</td>
<td>0.5</td>
<td>Soil (forest)</td>
</tr>
<tr>
<td>Landfills</td>
<td>Leachate</td>
<td>3</td>
<td>M-WWTP</td>
</tr>
<tr>
<td>Air pollution</td>
<td>Atmospheric deposition</td>
<td>600</td>
<td>Inland surface water</td>
</tr>
<tr>
<td>Air pollution</td>
<td>Atmospheric deposition</td>
<td>7000</td>
<td>Soil</td>
</tr>
</tbody>
</table>

Table A 2. Estimated emissions of TPP from different source categories

<table>
<thead>
<tr>
<th>Source</th>
<th>Name flow</th>
<th>Size flow (kg/year)</th>
<th>Released to</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processing of plastics</td>
<td>Diffusion to air</td>
<td>1.2</td>
<td>Indoor air</td>
</tr>
<tr>
<td>Processing of plastics</td>
<td>Wastewater</td>
<td>500</td>
<td>M-WWTP</td>
</tr>
<tr>
<td>Processing of plastics</td>
<td>Solid waste</td>
<td>580</td>
<td>Incineration</td>
</tr>
<tr>
<td>Households and industry</td>
<td>Influent wastewater</td>
<td>300 (100-500)</td>
<td>M-WWTP</td>
</tr>
<tr>
<td>Use of articles (LCD Screens)</td>
<td>Diffusion to air</td>
<td>3900</td>
<td>Indoor air</td>
</tr>
<tr>
<td>WWTP</td>
<td>Effluent wastewater</td>
<td>100 (30-200)</td>
<td>Surface water</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>40 (2-200)</td>
<td>Soil (filling material and agricultural soil)</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>20 (0.7-70)</td>
<td>Landfill</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>0.1 (0.006-0.6)</td>
<td>Incineration</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>20 (0.7-70)</td>
<td>Unknown</td>
</tr>
<tr>
<td>Landfill</td>
<td>Landfill leachate</td>
<td>7 (6-7)</td>
<td>Surface water</td>
</tr>
<tr>
<td>Landfill</td>
<td>Landfill leachate</td>
<td>7 (6-7)</td>
<td>Soil</td>
</tr>
<tr>
<td>Landfill</td>
<td>Landfill leachate</td>
<td>30 (30-40)</td>
<td>M-WWTP</td>
</tr>
</tbody>
</table>
Assessing the relative importance of emissions from articles of selected organic substances

### Table A 3. Estimated emissions of TBP from different source categories

<table>
<thead>
<tr>
<th>Source</th>
<th>Name flow</th>
<th>Size flow (kg/year)</th>
<th>Released to</th>
</tr>
</thead>
<tbody>
<tr>
<td>Use of concrete</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Households and industry</td>
<td>Influent wastewater</td>
<td>30 000 (10 000-90 000)</td>
<td>M-WWTP</td>
</tr>
<tr>
<td>Households and industry</td>
<td>Effluent wastewater</td>
<td>3 000 (30-10 000)</td>
<td>Surface water</td>
</tr>
<tr>
<td>Households and industry</td>
<td>Sewage sludge</td>
<td>20 (0.02-100)</td>
<td>Soil (filling material and agricultural soil)</td>
</tr>
<tr>
<td>Households and industry</td>
<td>Sewage sludge</td>
<td>9 (0.01-50)</td>
<td>Landfill</td>
</tr>
<tr>
<td>Households and industry</td>
<td>Sewage sludge</td>
<td>0.08 (0.0001-0.4)</td>
<td>Incineration</td>
</tr>
<tr>
<td>Households and industry</td>
<td>Sewage sludge</td>
<td>9 (0.01-50)</td>
<td>Unknown</td>
</tr>
<tr>
<td>Use of aircraft hydraulic fluids</td>
<td>Leakage of hydraulic fluid</td>
<td>5 000-20 000</td>
<td>Soil, wastewater, surface water</td>
</tr>
<tr>
<td>Use of articles</td>
<td>Diffusion from indoor air</td>
<td>0-3 400</td>
<td>Outdoor air</td>
</tr>
</tbody>
</table>

### Table A 4. Estimated emissions of MBT from different source categories.

<table>
<thead>
<tr>
<th>Source</th>
<th>Name flow</th>
<th>Size flow (kg/year)</th>
<th>Released to</th>
</tr>
</thead>
<tbody>
<tr>
<td>Use of tyres</td>
<td></td>
<td></td>
<td>Surface water</td>
</tr>
<tr>
<td>Use of tyres</td>
<td></td>
<td>450</td>
<td>Air</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Effluent wastewater</td>
<td>400 (&lt;100-1000)</td>
<td>Surface water</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sewage sludge</td>
<td>20 (&lt;2-100)</td>
<td>Soil (filling material and agriculture)</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sewage sludge</td>
<td>9 (&lt;1-50)</td>
<td>Landfills</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sewage sludge</td>
<td>0.08 (&lt;0.0009-0.4)</td>
<td>Incineration</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sewage sludge</td>
<td>10 (&lt;1-50)</td>
<td>Unknown</td>
</tr>
<tr>
<td>Landfills</td>
<td>Leachate</td>
<td>0.2</td>
<td>Surface water</td>
</tr>
<tr>
<td>Landfills</td>
<td>Leachate</td>
<td>0.2</td>
<td>Forest soil</td>
</tr>
<tr>
<td>Landfills</td>
<td>Leachate</td>
<td>2 (1-2)</td>
<td>M-WWTP</td>
</tr>
<tr>
<td>Air pollution</td>
<td>Atmospheric deposition</td>
<td>0.04</td>
<td>Inland surface water</td>
</tr>
<tr>
<td>Air pollution</td>
<td>Atmospheric deposition</td>
<td>5</td>
<td>Soil</td>
</tr>
</tbody>
</table>

### Table A 5. Estimated emissions of 8:2 FTOH from different source categories.

<table>
<thead>
<tr>
<th>Source</th>
<th>Name flow</th>
<th>Size flow (kg/year)</th>
<th>Released to</th>
</tr>
</thead>
<tbody>
<tr>
<td>M-WWTP</td>
<td>Effluent wastewater</td>
<td>7 (&lt;LOD-40)</td>
<td>Surface water</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sludge</td>
<td>2 (0.2-16)</td>
<td>Soil (filling material and agricultural soil)</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sludge</td>
<td>0.8 (0.1-7)</td>
<td>Landfills</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sludge</td>
<td>0.007 (0.0001-0.008)</td>
<td>Incineration</td>
</tr>
<tr>
<td>M-WWTP</td>
<td>Sludge</td>
<td>0.8 (0.1-7)</td>
<td>Unknown</td>
</tr>
<tr>
<td>Jackets</td>
<td></td>
<td>0.002</td>
<td>Air</td>
</tr>
<tr>
<td>Jackets</td>
<td></td>
<td>0.00001</td>
<td>Water</td>
</tr>
<tr>
<td>Indoor environment</td>
<td>Transport from indoor air</td>
<td>60 (10-300)</td>
<td>Outdoor air</td>
</tr>
</tbody>
</table>
Assessing the relative importance of emissions from articles of selected organic substances

Table A 6. Estimated emissions of diuron from different source categories

<table>
<thead>
<tr>
<th>Source</th>
<th>Name flow</th>
<th>Size flow (kg/year)</th>
<th>Released to</th>
</tr>
</thead>
<tbody>
<tr>
<td>Households and industry</td>
<td>Diffusion to air</td>
<td>1.3</td>
<td>Indoor air</td>
</tr>
<tr>
<td>Households and industry</td>
<td>Influent wastewater</td>
<td>60 (5-175)</td>
<td>M-WWTP</td>
</tr>
<tr>
<td>WWTP</td>
<td>Effluent wastewater</td>
<td>60 (&lt;20-140)</td>
<td>Surface water</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>&lt;0.6 – 8</td>
<td>Soil (filling material and agricultural soil)</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>&lt;0.5 – 3</td>
<td>Landfill</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>&lt;0.005 – 0.03</td>
<td>Incineration</td>
</tr>
<tr>
<td>WWTP</td>
<td>Sewage sludge</td>
<td>&lt;0.5 – 3</td>
<td>Unknown</td>
</tr>
<tr>
<td>Air pollution</td>
<td>Atmospheric deposition</td>
<td>0-2</td>
<td>Inland surface water</td>
</tr>
<tr>
<td>Air pollution</td>
<td>Atmospheric deposition</td>
<td>0-30</td>
<td>Soil</td>
</tr>
</tbody>
</table>
Appendix B: Data used for modelling

Model input

Table B 1. Estimated emissions from consumer articles (kg/year) in Sweden and Stockholm, used as input to the SMURF model. Releases to indoor air, outdoor air and wastewater were taken from direct calculations of emissions from products using the emission model described by Holmgren et al. (2012) (unpublished data from Holmgren and Haglund, Umeå University). Releases to surface water and soil were taken from the SFA calculations (see Appendix A), but the ranges were determined based on a confidence factor of 5.

<table>
<thead>
<tr>
<th>Substance</th>
<th>Indoor air</th>
<th>Outdoor air</th>
<th>Wastewater*</th>
<th>Surface water</th>
<th>Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sweden</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DINP</td>
<td>40** (8-200)</td>
<td>0.071 (0.014-0.35)</td>
<td>6.8×10⁻³⁰</td>
<td>100 (20-500)</td>
<td>4000 (200-20000)</td>
</tr>
<tr>
<td>TPP</td>
<td>11.5*** (2.3-57)</td>
<td>0.016 (0.003-0.081)</td>
<td>1.1×10⁻¹⁰</td>
<td>100 (20-500)</td>
<td>40 (8-200)</td>
</tr>
<tr>
<td>TBP</td>
<td>0.0016 (0.0003-0.008)</td>
<td>0</td>
<td>0</td>
<td>3100 (620-15500)</td>
<td>20 (4-100)</td>
</tr>
<tr>
<td>MBT</td>
<td>0.02 (0.004-0.1)</td>
<td>94 (19-470)</td>
<td>0</td>
<td>400 (80-2000)</td>
<td>20 (4-100)</td>
</tr>
<tr>
<td>8:2-FTOH</td>
<td>0.057 (0.011-0.29)</td>
<td>0.0024 (4×10⁻⁴-0.01)</td>
<td>1.2×10⁻⁶</td>
<td>7 (1.4-35)</td>
<td>2 (0.4-10)</td>
</tr>
<tr>
<td>Diuron</td>
<td>0.15 (0.03-0.75)</td>
<td>0</td>
<td>0</td>
<td>60 (12-300)</td>
<td>2 (0.4-10)</td>
</tr>
<tr>
<td><strong>Stockholm</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DINP</td>
<td>3.6 (0.72-18)</td>
<td>0.0064 (0.001-0.03)</td>
<td>6.1×10⁻³⁰</td>
<td>0-45</td>
<td>180 (36-900)</td>
</tr>
<tr>
<td>TPP</td>
<td>1.0 (0.21-5.2)</td>
<td>0.0015 (2.9×10⁻⁴-0.007)</td>
<td>9.9×10⁻¹²</td>
<td>9 (2-45)</td>
<td>3.6 (0.7-18)</td>
</tr>
<tr>
<td>TBP</td>
<td>1.4×10⁻⁴ (2.9×10⁻⁵-7.2×10⁻⁵)</td>
<td>0</td>
<td>0</td>
<td>280 (56-1395)</td>
<td>1.8 (0.36-9)</td>
</tr>
<tr>
<td>MBT</td>
<td>0.0018 (3.7×10⁻⁶-0.0091)</td>
<td>8.5 (1.7-42)</td>
<td>0</td>
<td>36 (7.2-180)</td>
<td>1.8 (0.36-9)</td>
</tr>
<tr>
<td>8:2-FTOH</td>
<td>0.0051 (0.001-0.025)</td>
<td>2.1×10⁻⁷ (4.2×10⁻⁸-0.001)</td>
<td>1.1×10⁻⁷</td>
<td>0.63 (0.12-0.35)</td>
<td>0.27 (0.05-1.35)</td>
</tr>
<tr>
<td>Diuron</td>
<td><strong>0.014 (0.0027-0.068)</strong></td>
<td>0</td>
<td>0</td>
<td>5.4 (1-27)</td>
<td>0.27 (0.05-1.35)</td>
</tr>
</tbody>
</table>

*releases to wastewater were not used as model input, only as comparison to model predicted outflow from indoor surfaces  **Emission figure includes estimated releases from vinyl flooring according to Holmgren et al. (2012) ***Emission figure includes estimated releases from LCD screens according to Holmgren et al. (2013b)
Assessing the relative importance of emissions from articles of selected organic substances

Table B 2. Physical-chemical properties at 25 degrees Celsius, estimated using the EPIWEB estimation software (USEPA, 2011). Background concentrations were taken from Westerdahl et al. (2012) and references therein.

<table>
<thead>
<tr>
<th></th>
<th>DINP</th>
<th>TPP</th>
<th>TBP</th>
<th>MBT</th>
<th>8:2 FTOH</th>
<th>Diuron</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight (g/mol)</td>
<td>419</td>
<td>326</td>
<td>266</td>
<td>167</td>
<td>464</td>
<td>233</td>
</tr>
<tr>
<td>Aqueous solubility (g/m³)</td>
<td>3.1×10⁻⁴</td>
<td>1.0</td>
<td>7.4</td>
<td>543</td>
<td>0.067</td>
<td>42</td>
</tr>
<tr>
<td>Vapor pressure (Pa)</td>
<td>6.8×10⁻⁶</td>
<td>6.29E⁻⁵</td>
<td>0.47</td>
<td>5.6×10⁻³</td>
<td>13</td>
<td>6.2×10⁻⁴</td>
</tr>
<tr>
<td>LogKow</td>
<td>8.6</td>
<td>4.7</td>
<td>4</td>
<td>2.9</td>
<td>5.6</td>
<td>2.7</td>
</tr>
<tr>
<td>Melting point (C)</td>
<td>-48</td>
<td>51</td>
<td>-79</td>
<td>180</td>
<td>10</td>
<td>160</td>
</tr>
<tr>
<td>deltaH solution (J/mol)</td>
<td>-10000</td>
<td>-10000</td>
<td>-10000</td>
<td>-10000</td>
<td>-10000</td>
<td>-10000</td>
</tr>
<tr>
<td>deltaH vaporization (J/mol)</td>
<td>1.2×10⁷</td>
<td>1.1×10⁷</td>
<td>7.3×10⁷</td>
<td>9.0×10⁶</td>
<td>6.0×10⁷</td>
<td>9.8×10⁷</td>
</tr>
<tr>
<td>Second order rate , kOH</td>
<td>2.3×10⁻¹¹</td>
<td>1.1×10⁻¹¹</td>
<td>7.9×10⁻¹¹</td>
<td>4.1×10⁻¹¹</td>
<td>4.2×10⁻¹²</td>
<td>1.1×10⁻¹¹</td>
</tr>
<tr>
<td>Water Rxn T1/2 (h)</td>
<td>2400</td>
<td>900</td>
<td>208</td>
<td>360</td>
<td>4320</td>
<td>900</td>
</tr>
<tr>
<td>Soil Rxn T1/2 (h)</td>
<td>1800</td>
<td>1800</td>
<td>416</td>
<td>720</td>
<td>8640</td>
<td>1800</td>
</tr>
<tr>
<td>Sediment Rxn T1/2 (h)</td>
<td>8100</td>
<td>8100</td>
<td>1.87E+03</td>
<td>3240</td>
<td>38900</td>
<td>8100</td>
</tr>
<tr>
<td>Background concentration in air (ng/m³)</td>
<td>0.25*</td>
<td>12</td>
<td>0.28</td>
<td>&lt;0.0005*</td>
<td>0.014</td>
<td>&lt;0.0005*</td>
</tr>
</tbody>
</table>

*Represents detection limit
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Monitoring data used for model evaluation

For TPP and TBP, concentrations in fish were used to estimate surface water concentrations. Measured concentrations in perch in lakes near Stockholm were determined to 32-150 ng/g lw for TPP and to 14 - 4900 ng/g lw for TBP (Sundkvist and Haglund, 2009). Using a fat content of 0.5 % and a BCF of 74 and 69.6 L/kg ww for TPP and TBP, respectively (calculated using the Arnot-Gobas method, EPIWEB software, USEPA (2011)), the corresponding water concentrations were calculated to be 2-10 ng/L and 1-350 ng/L for TPP and TBP, respectively.

Table B 3. Monitoring data (median + range) used for model evaluation and their references.

<table>
<thead>
<tr>
<th>Substance</th>
<th>Indoor air (ng/m^3)</th>
<th>Indoor dust (ng/g)</th>
<th>Outdoor air (ng/m^3)</th>
<th>Urban surface water (ng/L)</th>
<th>Urban sediment (ng/g dw)</th>
<th>Urban soil (ng/g dw)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DINP</td>
<td>2.1 (&lt;2.4-6)^a</td>
<td>4.1×10^4 (-4.0×10^4 - 4.1×10^7)^b</td>
<td>8.5 (0.66-50)^c</td>
<td>n.a.</td>
<td>2000 (2000-3200)^c</td>
<td>n.a.</td>
</tr>
<tr>
<td>TPP</td>
<td>&lt;3.1 (n.d.-25)^d,e</td>
<td>2800 (100-32000)^a</td>
<td>n.a.</td>
<td>6^-f</td>
<td>n.a.</td>
<td>n.a.</td>
</tr>
<tr>
<td>TBP</td>
<td>10.8 (n.d.-320)^d,e</td>
<td>2300 (100-6200)^y</td>
<td>n.a.</td>
<td>175^-f</td>
<td>n.a.</td>
<td>n.a.</td>
</tr>
<tr>
<td>MBT^g</td>
<td>n.a.</td>
<td>n.a.</td>
<td>&lt;0.2 &lt;0.05-0.3</td>
<td>&lt;10 (&lt;3-100)</td>
<td>&lt;20 (&lt;0.8-70)</td>
<td>&lt;0.7 (&lt;0.6-0.8)</td>
</tr>
<tr>
<td>8:2-FTOH**</td>
<td>5.2 (0.92-25)^h</td>
<td>63 (9-4670)^j</td>
<td>0.12 (0.08-0.37)^i</td>
<td>n.a.</td>
<td>n.a.</td>
<td>n.a.</td>
</tr>
<tr>
<td>Diuron</td>
<td>n.a.</td>
<td>n.a.</td>
<td>n.a.</td>
<td>22 (10-50)^j</td>
<td>0.1 (0.07-0.24)^k</td>
<td>15 (10-15)^l</td>
</tr>
</tbody>
</table>


*Estimated from fish data

**No Swedish data found. Data taken from Norwegian and Canadian studies.
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References


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Appendix C: Additional model results

Estimating the contribution of the indoor environment to TBP in M-WWTP influents

The contribution of TBP releases to M-WWTPs from indoor dust was assessed, using Henriksdal as example WWTP. The annual water inflow at Henriksdal is 10440 m³/h or 9.1×10⁷ m³/year. The ingoing concentration of TBP at Henriksdal has been measured to 9.95 µg/l on average (n=2) which corresponds to an annual inflow of about 900 kg TBP. Because of the limited partitioning to indoor surfaces, the predicted outflow from the indoor environment in Stockholm via wet removal (i.e. mopping of floors etc.) is also small, only 0.0006 kg/year, or 0.001 kg/year if dry removal is included. Assuming that this amount goes directly to Henriksdal, suggests that the indoor environment contributes by about 0.0001 % to the total incoming amounts of TBP to the M-WWTPs.