Evaluation of using mobility of chemicals in the environment to fulfil bioaccumulation criteria of the Stockholm Convention

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Authors: M J Crookes and P Fisk

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Conclusions drawn and recommendations made in this report represent the unbiased view of Peter Fisk Associates on the basis of the data presented and obtained.

The signature below confirms that this version of the report is complete and final.

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Signed on behalf of Peter Fisk Associates Ltd by authorised signatory:

........................................................................................................

Name ......................................................................................

Position ...................................................................................

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**Executive summary**

This report considers how the objectives of the Stockholm Convention on Persistent Organic Pollutants (POPs) can be related to measures of mobility; particularly as a screening criterion for potential new POPs.

In the context of identification of such chemicals, the criteria for POP substances in Annex D of the Stockholm Convention are largely based on the properties of well-known organic chemicals that have caused global pollution problems in the past. These include chemicals such as the polychlorinated biphenyls (PCBs) and a number of other organochlorine substances (including pesticides DDT, ‘drins’ and lindane). The properties of these substances mean that they persist for long periods in environmental media, accumulate in food chains, and are capable of being transported long distances (largely by atmospheric distribution) and then being redeposited. These substances can be considered to show “classic POPs” behaviour.

One focus for policy makers and regulators is on the robustness of Annex D screening criteria to identify substances that are of concern. The perfluorinated compounds, pentadecafluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS), are cases in point. These substances persist for very long periods in the environment and are capable of being transported and distributed globally through water or adsorbed onto particulates. They are also known to be accumulated in the bodies of animals and in the tissues of human beings. However, the current screening for bioaccumulation would not necessarily identify PFOA and PFOS against the standard Annex D criteria under c(i). This is, in part, because PFOS and PFOA are both highly soluble, and because their accumulation in tissue is not as a result of uptake into lipid but rather their action as surfactants and their binding to proteins. It is the persistence of these substances in the environment combined with their residence time in living organisms that makes them of concern; but it is their mobility in the environment (particularly the aquatic environment) that allows very wide distribution far from source. Substances that are both persistent and mobile in the environment have the potential to be transported long distances from the point of emission. If such substances accumulate over time in remote regions they can reach levels that may have effects on both ecosystems and human health.

In terms of the criteria for bioaccumulation, traditional “bioaccumulative” substances would be captured by Annex D criterion c(i), i.e. substances with a high affinity for lipids and which accumulate significantly in lipid tissues. However, the Annex D criterion c(ii) allows other indications of concern to be considered in relation to bioaccumulation. The purpose of the current report is to investigate whether and how measures of mobility can be used within the bioaccumulation criterion c(ii) within Annex D in this context.

The mobility of substances in water has recently been highlighted by various authors and regulatory authorities as an issue in the context of drinking water resources. The current study has used the criteria proposed in the drinking water context as a starting point and has investigated whether these mobility-based concerns can be extended to bioaccumulation-based concerns in relation to the criteria in Annex D of the Stockholm Convention.

The study has found that, by taking into account the time to reach a certain body burden, a wider range of screening criteria than currently included in the Stockholm Convention is needed to screen for POP substances. The current Stockholm Convention criteria are appropriate for
substances which have high bioconcentration/bioaccumulation factors and thus reach relatively high body burdens over relatively short time periods. However, a wider range of criteria is necessary to capture mobility-based concerns for substances that have lower bioconcentration/bioaccumulation factors but which may accumulate over longer time periods. This includes consideration of how the substances are transported (e.g. mainly via water, mainly via air or a combination of both), and consideration of persistence over longer time-scales than currently included in the Stockholm Convention criteria. These factors need to be considered in an integrated manner and so mobility alone (as has been proposed for drinking water) is not a good marker in relation to the POPs context.

Based on the analysis carried out, the new additional criteria below are proposed for screening of substances that may be of concern in relation to their mobility within the framework set out in Annex D of the Stockholm Convention. These criteria could be considered under c(ii) of Annex D. The criteria proposed have been validated using substances that do not meet the current Stockholm Criteria for bioaccumulation, but which have been agreed to be POPs.

- **Persistent, Mobile, and Toxic (PMT) substances with log \(K_{ow}\) < 5 or log \(K_{oc}\) < 5 with log \(K_{aw}\) in the range 0 to -3.
  - Log \(K_{ow}/log K_{oc}\) and log \(K_{aw}\) in these ranges indicate that the substance may be mobile in water and air.
  - The persistence should be based on the degradation half-life in water, sediment or soil and be related to the environmental compartment in which, or through which, the substance is considered to be mobile. This will need to be considered case-by-case taking into account the properties of the substance. For example, substances with relatively low log \(K_{ow}\) values (e.g. log \(K_{ow}\) < 3) would be expected to be present mainly in the surface water phase but for higher log \(K_{ow}\) values they may increasingly be present in the sediment or soil phase. The half-life in water, sediment or soil should be demonstrably >1 year.
  - It is important to note that transport via the air may also be important for some members of this group and so it is necessary to consider the overall persistence in an integrated manner. When the half-life in air is long (>50 days) it may be appropriate to reduce the half-life in water, sediment or soil to 180 days.

- **Persistent, Mobile and Toxic (PMT) substances with log \(K_{ow}\) < 5 or log \(K_{oc}\) < 5 with log \(K_{aw}\) in the range < -3.
  - Log \(K_{ow}/log K_{oc}\) and log \(K_{aw}\) in these ranges indicate that the substance may be mobile in water.
  - The persistence should be based on the degradation half-life in water, sediment or soil and be related to the environmental compartment in which, or through which, the substance is considered to be mobile. As above, this will need to be considered case-by-case taking into account the properties of the substance. The half-life in water, sediment or soil should be demonstrably >1 year.
  - When the half-life in air is long (>50 days) it may be appropriate to reduce the half-life in water, sediment or soil to 180 days.

- **Extremely persistent substances.** This group would consist of substances which have a low bioaccumulation potential (e.g. a BCF <<5,000 l/kg) but which show extreme persistence in a relevant environmental media (half-life >>1 year).
It is important to note that mobility-based concerns are a result of a combination of a number of factors and it is difficult to capture all of these factors within simple numerical criteria. Therefore, the screening criteria developed should be seen as the starting point for identifying potential candidates for further evaluation. Proper assessment of mobility based concerns requires understanding of the actual modes of transport and the interaction of the various partitioning and degradation processes that may occur, and needs to be considered on a case-by-case basis by using in-depth modelling and assessment methods. Such assessment approaches are beyond the scope of the current project.
## Glossary

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTD</td>
<td>Characteristic travel distance. The CTD is an estimate of the distance from a point source at which the concentration of a chemical will have dropped to 38% of its initial concentration.</td>
</tr>
<tr>
<td>Distribution coefficient</td>
<td>Similar to partition coefficient but for ionisable substances. Ratio of concentrations of all forms (non-ionised and ionised) substance between two media (e.g. octanol-water).</td>
</tr>
<tr>
<td>DNEL</td>
<td>Derived-no-adverse-effect-level.</td>
</tr>
<tr>
<td>$D_{ow}$</td>
<td>Octanol-water distribution coefficient.</td>
</tr>
<tr>
<td>Half-life</td>
<td>The time taken for a concentration to fall to half of its original concentration.</td>
</tr>
<tr>
<td>$K_{aw}$</td>
<td>Air-water partition coefficient.</td>
</tr>
<tr>
<td>$K_{oa}$</td>
<td>Octanol-air partition coefficient.</td>
</tr>
<tr>
<td>$K_{oc}$</td>
<td>Organic carbon-water partition coefficient.</td>
</tr>
<tr>
<td>$K_{ow}$</td>
<td>Octanol-water partition coefficient.</td>
</tr>
<tr>
<td>Log $K_{oa}$</td>
<td>Logarithm (base 10) of the octanol-air partition coefficient.</td>
</tr>
<tr>
<td>Log $K_{oc}$</td>
<td>Logarithm (base 10) of the organic carbon-water partition coefficient.</td>
</tr>
<tr>
<td>Log $D_{ow}$</td>
<td>Logarithm (based 10) of the octanol-water distribution coefficient.</td>
</tr>
<tr>
<td>Log $K_{ow}$</td>
<td>Logarithm (base 10) of the octanol-water partition coefficient.</td>
</tr>
<tr>
<td>Log $K_{aw}$</td>
<td>Logarithm (base 10) of the air-water partition coefficient.</td>
</tr>
<tr>
<td>LRTP</td>
<td>Long-range transport potential.</td>
</tr>
<tr>
<td>M</td>
<td>Mobile.</td>
</tr>
<tr>
<td>NOEC</td>
<td>No-observed effect concentration.</td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>Ratio of concentrations of a (non-ionised) substance between two media (e.g. octanol-water, air-water, octanol-air, organic carbon-water).</td>
</tr>
<tr>
<td>P</td>
<td>Persistent.</td>
</tr>
<tr>
<td>Pov</td>
<td>Overall environmental persistence. Pov is an estimate of the overall residence time (in days) of the substance in a model system.</td>
</tr>
<tr>
<td>PBT</td>
<td>Persistent, bioaccumulative and toxic.</td>
</tr>
<tr>
<td>pH</td>
<td>The negative logarithm (base 10) of the hydrogen ion concentration.</td>
</tr>
<tr>
<td>pKa</td>
<td>The negative logarithm (base 10) of the acid dissociation constant.</td>
</tr>
<tr>
<td>PM</td>
<td>Persistent and mobile.</td>
</tr>
<tr>
<td>Acronym</td>
<td>Definition</td>
</tr>
<tr>
<td>----------</td>
<td>---------------------------------------------------------------------------</td>
</tr>
<tr>
<td>PMT</td>
<td>Persistent, mobile and toxic.</td>
</tr>
<tr>
<td>POP</td>
<td>Persistent Organic Pollutant.</td>
</tr>
<tr>
<td>T</td>
<td>Toxic.</td>
</tr>
<tr>
<td>TE</td>
<td>Transport efficiency. The TE is an estimate of the percentage of emitted substance that is deposited to surface media after transport away from the region of release.</td>
</tr>
<tr>
<td>UVCB</td>
<td>Substances of unknown or variable composition, complex reaction products or biological materials.</td>
</tr>
<tr>
<td>vM</td>
<td>Very mobile.</td>
</tr>
<tr>
<td>vP</td>
<td>Very persistent.</td>
</tr>
<tr>
<td>vPvB</td>
<td>Very persistent, very bioaccumulative.</td>
</tr>
<tr>
<td>vPvM</td>
<td>Very persistent, very mobile.</td>
</tr>
</tbody>
</table>
Evaluation of using mobility of chemicals in the environment to fulfil the bioaccumulation criteria of the Stockholm Convention

1. Background

The Stockholm Convention on Persistent Organic Pollutants (POPs) is a global treaty which aims “to protect human health and the environment from chemicals that remain intact in the environment for long periods, become widely distributed geographically, accumulate in the fatty tissues of humans and wildlife, and have harmful impacts on human health or on the environment”.

The Convention sets out information requirements and screening criteria for identification of POPs in Annex D (Stockholm Convention, 2009). Annex D sets down the criteria for identification of POPs based on quantified threshold values covering the potential for persistence, bioaccumulation, long range transport, and adverse effects.

This report considers how ‘mobility’ may relate to the objectives of the Stockholm Convention, including as screening criteria for potential POPs and proposes how mobility in water could be used for identification of substances that may be of concern in relation to their mobility within the framework set out in Annex D.

1.1 Further consideration of the Annex D criteria

Annex D of the Convention outlines information requirements and screening criteria for identifying POPs. These are reproduced below.

a) Chemical identity:
   i. Names, including trade name or names, commercial name or names and synonyms, Chemical Abstracts Service (CAS) Registry number, International Union of Pure and Applied Chemistry (IUPAC) name; and
   ii. Structure, including specification of isomers, where applicable, and the structure of the chemical class;

b) Persistence:
   i. Evidence that the half-life of the chemical in water is greater than two months, or that its half-life in soil is greater than six months, or that its half-life in sediment is greater than six months; or
   ii. Evidence that the chemical is otherwise sufficiently persistent to justify its consideration within the scope of this Convention;

c) Bioaccumulation:

i. Evidence that the bio-concentration factor or bio-accumulation factor in aquatic species for the chemical is greater than 5,000 or, in the absence of such data, that the log $K_{ow}$ is greater than 5;

ii. Evidence that a chemical presents other reasons for concern, such as high bio-accumulation in other species, high toxicity or ecotoxicity; or

iii. Monitoring data in biota indicating that the bio-accumulation potential of the chemical is sufficient to justify its consideration within the scope of this Convention;

d) Potential for long-range environmental transport:

i. Measured levels of the chemical in locations distant from the sources of its release that are of potential concern;

ii. Monitoring data showing that long-range environmental transport of the chemical, with the potential for transfer to a receiving environment, may have occurred via air, water or migratory species; or

iii. Environmental fate properties and/or model results that demonstrate that the chemical has a potential for long-range environmental transport through air, water or migratory species, with the potential for transfer to a receiving environment in locations distant from the sources of its release. For a chemical that migrates significantly through the air, its half-life in air should be greater than two days; and

e) Adverse effects:

i. Evidence of adverse effects to human health or to the environment that justifies consideration of the chemical within the scope of this Convention; or

ii. Toxicity or ecotoxicity data that indicate the potential for damage to human health or to the environment.

In the context of identification of such chemicals, criteria for POP substances have been based on the properties of well-known organic chemicals, such as the polychlorinated biphenyls (PCBs) and a number of other organochlorine substances (including pesticides DDT, ‘drins’ and lindane), that have caused global pollution problems in the past. The properties of these substances mean that they persist for long periods in environmental media, accumulate in food chains, and are capable of being transported long distances (largely by atmospheric distribution) and then being redeposited. The application of these criteria (and of course understanding of use patterns and releases to the environment), has allowed many other substances that are of global concern as pollutants – for example some brominated flame retardants - to be identified and controlled under the Convention. These substances exhibit ‘classic POP’ behaviour, meeting the criteria and being measured globally in environmental compartments including the tissue of living organisms.

One focus for policy makers and regulators is on the robustness of screening criteria, to identify substances that are POPs. The perfluorinated compounds, pentadecafluoroctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS), are cases in point. These substances persist for very long periods in the environment and are capable of being transported and distributed globally through water or adsorbed onto particulates. They are also known to be accumulated in the bodies of animals and in the tissues of human beings. However, the screening for bioaccumulation (derived largely on the basis of the properties of the classic POPs as described above e.g. BCF values) would not necessarily identify PFOA and PFOS against the standard Annex D criteria under c(i). This is, in part, because PFOS and PFOA are both highly soluble, and because their accumulation in tissue is not as a result of uptake into lipid (predicted by affinity for octanol versus water ($K_{ow}$)) but rather their action as surfactants and their binding
to proteins. It is the persistence of these substances in the environment combined with their residence time in living organisms that makes them of concern; but it is their mobility in the environment (particularly the aquatic environment) that allows very wide distribution far from source.

Prediction of accumulation in organisms and the magnification of concentrations up the food chain (whereby predator species can exhibit far greater concentrations in their tissues than their prey and the environments in which they live) is an important metric, but one which is difficult to predict for the perfluoro substances. Furthermore, lack of the data specified under Annex D (Log $K_{ow}$ or BCF) can make the discussions at Persistent Organic Pollutants Review Committee (POPRC) meetings more challenging with a possible result that conclusions take longer to be reached for these kinds of substances.

In terms of the criteria for bioaccumulation, traditional “bioaccumulative” substances would be captured by criterion c(i), i.e. substances with a high affinity for lipids and which accumulate significantly in lipid tissues. However, the criterion c(ii) allows other indications of concern to be considered in relation to bioaccumulation. The purpose of the current report is to investigate whether and how measures of mobility can be used within the bioaccumulation criterion c(ii) within Annex D in this context.

It is also important to note that Article 8 of the Convention indicates that the screening criteria in Annex D should be applied “in a flexible and transparent way, taking all information provided into account in an integrative and balanced manner”. This means that criterion c(ii) should be considered in an integrated manner with the other criteria from Annex D.

The Annex D criteria therefore link persistence, bioaccumulation and toxicity as the criteria of concern which, in combination with a potential for long-range transport, are used to identify POPs. The question remains as to whether other factors, not necessarily directly related to bioaccumulation potential, could be considered in relation to the bioaccumulation criterion, which also give rise to similar levels of concerns and hence could be used to identify POPs.

### 2. Mobility-based concerns

Outside of the specific processes of the Stockholm Convention, the mobility of substances in water has already been identified by various authors and regulatory authorities, including the German Federal Environment Agency (Umwelt Bundesamt – ‘UBA’), as a serious concern with potential implications for human health. These concerns have been recently highlighted as an issue in the context of drinking water resources (UBA, 2017; Reemtsma et al., 2016; Neuman (2017).

Reemtsma et al. (2016) noted that regulations based on persistent, bioaccumulative and toxic (PBT) properties of substances are not necessarily effective for the protection of drinking water quality as bioaccumulative organic substances tend to be relatively non-polar, lipophilic and hydrophobic substances with limited solubility in water. These properties mean that they can be removed readily from the water phase during water treatment and by sorption processes in the environment. In terms of raw water quality, substances that are both persistent and mobile may be of concern as they can be more polar, with relatively high water solubilities and so are
not easily removed from water by sorption processes. This combination of properties means that persistent and mobile substances may end up in drinking water in greater quantities than standard PBT substances.

Reemtsma et al. (2016) named methyl tertiary butyl ether (MTBE), ethylene diamine tetraacetic acid (EDTA), short-chain perfluoralkyl acids (PFAAs) and tris(2-chloroethyl)phosphate (TCEP) as examples of persistent and mobile organic chemicals that are widely found in raw waters used for production of drinking water.

Although the focus of the UBA (2017) and Reemtsma et al. (2016) studies was on drinking water derived from freshwater sources including groundwater aquifers, similar considerations can be applied to any aquatic environment, including pristine and remote freshwater or marine environments.

Substances that are both persistent and mobile in the environment have the potential to be transported long distances from the point of emission. If such substances accumulate over time in remote regions they can reach levels that may have effects on both ecosystems and human health. In this context it is important to understand that “accumulate” is a broader term than bioaccumulation as it covers accumulation of substances in environmental media such as water or sediment rather than being limited to only living organisms.

As far as the authors of this present report are aware there is no agreed regulatory definition of mobility in water. As an equivalent definition, Annex II of the REACH Regulation\(^2\) defines mobility in soil as follows:

> “Mobility in soil is the potential of the substance or the components of a mixture, if released to the environment, to move under natural forces to the groundwater or to a distance from the site of release.”

and

> “Information on mobility in soil can be determined from relevant mobility data such as adsorption studies or leaching studies, known or predicted distribution to environmental compartments, or surface tension. For example, \(K_{oc}\) values can be predicted from octanol/water partition coefficients (\(K_{ow}\)). Leaching and mobility can be predicted from models.”

Reemtsma et al. (2016) suggested that two properties that could possibly be used to quantify mobility in water are water solubility and sorption tendency. They argued that the molecules which are most mobile in water are those in which solvation by water is energetically more favourable than sorption to environmental solids, i.e. the most mobile substances have relatively high water solubilities and do not adsorb strongly to suspended solids or sediments.

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For non-polar organic compounds, the octanol-water partition coefficient (K<sub>ow</sub>) can be used as an indicator of a substance’s sorption tendency, with the sorption tendency generally increasing as the K<sub>ow</sub> increases. However, K<sub>ow</sub> may not be a good indicator of the sorption tendency of some groups of chemicals such as those with specific polar and non-specific apolar interactions with bulk phases, in particular, ionic and dissociating compounds (Reemtsma et al., 2016). For ionic and dissociating substances Reemtsma et al. (2016) suggested that the octanol-water distribution coefficient (D<sub>ow</sub>) could be used as an alternative simplistic indicator. For organic acids, Reemtsma gave the following well-known equation for the pH-dependency of the D<sub>ow</sub>.

\[
D_{ow} = \frac{K_{ow}}{1 + 10^{pH - pKa}}
\]

Where

- \( D_{ow} \) = octanol-water distribution coefficient
- \( K_{ow} \) = octanol-water partition coefficient
- \( pKa \) = -log<sub>10</sub> of the acid dissociation constant
- \( pH \) = -log<sub>10</sub> of the hydrogen ion concentration in the environmental media

It is possible to derive similar equations for bases and amphoteric substances, as has been well-described in scientific literature.

### 2.1 Persistent, mobile, toxic (PMT) and very persistent, very mobile (vPvM) criteria

The UBA (2017) report on protection of drinking water provides a proposal for criteria for identifying Persistent, Mobile and Toxic (PMT) and very Persistent, very Mobile (vPvM) substances that have been registered under the EU REACH Regulation. Similar proposals are also reported in Neumann (2017). The aim of these criteria is to identify substances that pose a hazard to the sources of drinking water.

The UBA (2017) criteria are discussed below. As noted above, these criteria were derived with a focus on identifying substances hazardous to sources of drinking water. Where adaptations/additional considerations may be relevant to application of these criteria within the context of the Stockholm Convention, these are noted.

Persistence criterion proposed by UBA (2017)

A substance fulfils the persistence criterion (P) if:

- a) the degradation half-life in marine water at 9°C is higher than 60 days; or
- b) the degradation half-life in freshwater or estuarine water at 12°C and pH 4-9 is higher than 40 days; or
- c) the degradation half-life in marine sediment at 9°C is higher than 180 days; or
- d) the degradation half-life in fresh or estuarine water sediment at 12°C and pH 4-9 is higher than 120 days; or
- e) the degradation half-life in soil at 12°C and pH 4-9 is higher than 120 days.

A substance fulfils the very persistent criterion (vP) if:
a) the degradation half-life in marine (9°C), fresh or estuarine water (12°C and pH 4-9) is higher than 60 days; or
b) the degradation half-life in marine (9°C), fresh or estuarine water sediment (12°C and pH 4-9) is higher than 180 days; or
c) the degradation half-life in soil (12°C and pH 4-9) is higher than 180 days.

Note: as indicated in Section 1, the Stockholm Convention has its own criteria for persistence. Lower temperatures may apply in remote Arctic/Antarctic regions.

Mobility criterion proposed by UBA (2017)

A substance fulfils the mobile criterion (M) if:

a) the highest water solubility is ≥0.15 mg/l and the lowest log K_{oc} is ≤4.0 at environmentally relevant pH range of 4-9 and at a temperature of 12°C; or
b) in the absence of log K_{oc} data, the highest water solubility is ≥0.15 mg/l and the lowest log D_{ow} or log K_{ow} is ≤4.0 at environmentally relevant pH range of 4-9 and at a temperature of 12°C.

A substance fulfils the very mobile criterions (vM) if:

a) the highest water solubility is ≥0.15 mg/l and the lowest log K_{oc} is ≤3.0 at environmentally relevant pH range of 4-9 and at a temperature of 12°C; or
b) in the absence of log K_{oc} data, the highest water solubility is ≥0.15 mg/l and the lowest, log D_{ow} or log K_{ow} is ≤3.0 at environmentally relevant pH range of 4-9 and a temperature of 12°C.

Note: Lower temperatures may apply in remote Arctic/Antarctic regions.

Toxicity criterion proposed by UBA (2017)

A substance fulfils the toxicity criterion (T) if:

a) the long-term no-observed effect concentration (NOEC) or EC_{10} for marine or freshwater organisms is less than 0.01 mg/l; or
b) the substance meets the criteria for classification as carcinogenic (category 1A, 1B or 2), germ cell mutagenic (category 1A, 1B or 2), or toxic for reproduction (category 1A, 1B, or 2) according to Regulation EC No 1272/2008; or
c) there is other evidence of chronic toxicity, as identified by the substance meeting the criteria for classification: specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) according to Regulation EC No 1272/2008; or
d) the substance meets the criteria for classification as “additional category for effects on or via lactation”, according to Regulation EC No 1272/2008; or
e) the Derived-No-Adverse-Effect-Level (DNEL) is ≤9 μg/kg/d (oral, long term, general population); or

3 D_{ow} is the pH-dependent octanol-water partition coefficient. For neutral substances, the octanol water partition coefficient, K_{ow} is used.
f) the substance acts as an endocrine disruptor in humans and/or wildlife species according to the WHO/IPCS definition of an endocrine disruptor. This is always the case if a substance can be identified as an endocrine disruptor for human health and/or the environment according to the criteria laid down in the draft of COMMISSION REGULATION (EU) …/… of XXX for setting out scientific criteria for the determination of endocrine disrupting properties and amending Annex II to Regulation (EC) 1107/2009.

Note: the Stockholm Convention has its own criteria for toxicity/adverse effects.

The criteria for mobility consider transport to be mainly via water. However, within the Stockholm Convention, transport via other mechanisms, for example, the air, also needs to be considered. For example, it is possible for chemicals to volatise and deposition into water a number of times forming a ‘leap-frog’ effect spanning long range transport.

2.2 Numbers of substances potentially meeting the M or vM criteria

In order to understand the potential number and types of substances that could meet the M or vM criteria proposed by UBA, a search of the OECD eChemPortal\(^4\) has been undertaken by the authors of this report for substances with the following properties.

**M**

- Water solubility between 0.15 mg/l and 1,000,000 mg/l; and
- log \(K_{ow}\) between \(^5\) -10 and 4 and;
- the results of biodegradation screening tests were either “not inherently biodegradable” or “under test conditions no biodegradation observed”.

**vM**

- Water solubility between 0.15 mg/l and 1,000,000 mg/l; and
- log \(K_{ow}\) between -10 and 3 and;
- the results of biodegradation screening tests were either “not inherently biodegradable” or “under test conditions no biodegradation observed”.

The approximate numbers of substances found with these combinations of properties were as follows.

- **M** – approximately 970 substances.
- **vM** – approximately 830 substances.

It is important to note that many more substances would have been obtained if less stringent cut-offs had been applied to the results of the biodegradation screening tests.

The number of substances potentially meeting the vM criteria is of particular interest. This is because there is no consideration of toxicity included in the proposal for vPvM and the more biodegradable substances (i.e. those that were readily or inherently biodegradable) were

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\(^4\) [https://www.echemportal.org/echemportal/propertysearch/page.action?pageID=0](https://www.echemportal.org/echemportal/propertysearch/page.action?pageID=0) The search was undertaken on the 7th February 2018.

\(^5\) A log \(K_{ow}\) of -10 is meaningless but was used in the search to ensure that all substances with reported negative log \(K_{ow}\) values would be found.
screened out by the search method used. The number of substances found here is therefore a good indication of the lower limit of the number of substances that would potentially screen for vPvM using the UBA criteria.

Most of the substances found using this approach are substances that have been registered in the EU under the REACH Regulation with data sets available through the European Chemicals Agency (ECHA) dissemination database. The search was carried out on the 7th February 2018; further substances with these properties may have been added to the ECHA database since the search was carried out.

UBA (2018) recently considered the PMT properties of 167 substances that have been registered under the REACH Regulation. The criteria used were modified criteria proposed by Kalberlah et al. (2014). These criteria were broadly similar to the UBA (2017) criteria discussed in Section 2.1.

The 167 substances considered in the UBA (2018) report were preselected based on a high likelihood of their occurrence in raw water (156 substances modelled as persistent and mobile with a high potential to be emitted to the environment, along with 11 substances that were already considered as PM or PMT substances by Kalberlah et al. 2014).

Of the 167 preselected substances, 9 substances were assessed as PMT and 20 substances were assessed as PM substances with suspected T. A further 105 substances were suspected to meet the PMT criteria, but this could not be confirmed with the data available. Considerable data gaps were found amongst the substances considered, particularly relating to mobility and toxicity, and this limited the accuracy of the assessments that could be made.

A further study of the PMT and vPvM properties has become available very recently (NGI, 2018). The study was based on 9,741 identifiable organic substances that had been registered under REACH as of May 2017. Comparison against the proposed UBA (2017) criteria revealed around 240 substances with sufficient weight of evidence to potentially meet the criteria for PMT and vPvM.

### 2.3 Other approaches

A recent report has looked into the case for regulating substances solely on the basis of their persistence in the environment (European Commission, 2017). The study argued that very persistent (vP) substances can remain in the environment for indefinite periods of time and may eventually reach concentrations that result in continuous exposures similar to those that can occur through bioaccumulation, resulting in harmful effects to health, environment and natural resources. Such contamination could be poorly reversible for vP substances.

The European Commission (2017) report did not specifically define new criteria for identification of vP substances but rather referred to the REACH vP criteria of a half-life in water of more than 60 days or a half-life in soil or sediment of more than 180 days.

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6 https://echa.europa.eu/information-on-chemicals/registered-substances

7 Registered substances that were either inorganic or complex UVCB substances (substances of Unknown or Variable composition, Complex reaction products or Biological materials) were excluded.
3. Mobility and the relationship with the POPs criteria

In order to develop useful criteria for mobility in relation to the aims of the Stockholm convention it is first necessary to consider how mobility relates to the current POPs criteria.

Although mobility could be considered as a relevant consideration in relation to bioaccumulation under clause c(ii) of the Annex D criteria (see Section 1.1), it is also a relevant consideration for two of the other current POPs criteria: b) persistence and d) long-range environmental transport. Therefore, it is important to consider all three aspects when developing suitable criteria for mobility.

The criteria proposed by UBA were developed specifically for identifying substances that may cause concerns for drinking water contamination, including ground water and surface water sources. The criteria proposed by UBA consider persistence in terms of degradation in water, sediment or soil. However, in terms of the aims of the Stockholm convention, other removal or partitioning processes may be important. An important case is volatile substances: on release to the environment, these may move rapidly from the water or soil phase to the air phase and undergo subsequent transport. If the properties of the substance are such that long-range transport could occur, then this would provide a mechanism for widespread transport other than just by the water phase. This suggests that volatility should also be considered in relation to any mobility consideration for the Stockholm Convention.

3.1 Relationship of the UBA Criteria with long-range transport

In order to further investigate the relationship of the criteria proposed in UBA (2017) with persistence and the potential for long-range transport and subsequent accumulation in remote regions, we have undertaken a number of modelling approaches.

3.1.1 OECD P_{OV} and LRTP Screening Tool, Version 2.2

The OECD P_{OV} and LRTP Screening Tool (OECD, 2009) can be used for screening level assessments of the overall environmental persistence (P_{OV}) and long-range transport potential (LRTP) of organic substances. The model is described in a paper by Wegmann et al. (2009).

The main outputs from the model are the P_{OV}, characteristic travel distance (CTD, km) and the transport efficiency (TE, %). The P_{OV} is an estimate of the overall residence time (in days) of the substance in the entire model system and can be calculated within the model for releases to air, water or soil. The CTD is an estimate of the distance from a point source at which the concentration of a chemical will have dropped to 38% of its initial concentration, and can be calculated within the model for releases to air or water. The CTD can be taken as a measure of the “mobility” of a substance in the environment. The TE is an estimate of the percentage of emitted substance that is deposited to surface media after transport away from the region of release, and can be calculated within the model for releases to air, water or soil.

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\[ This represents approximately 1/e of the original concentration.\]
The tool requires only limited substance property data (essentially an estimated degradation half-life in soil, water and air along with octanol-water and air-water partition coefficients) which makes it ideal for investigating the relative effects of these properties on the long-range transport metrics calculated by the model.

The OECD Screening Tool was used to explore the properties of chemicals that may support long range transport, based around the criteria proposed in UBA (2017). In order to do this, the model was run several times varying the input data within the ranges shown in Table 3.1

Range of input data used for modelling around the UBA (2017) criteria

<table>
<thead>
<tr>
<th>Model input data</th>
<th>Range investigated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>200 g/mole (same value used in all model runs)</td>
</tr>
<tr>
<td>$\log K_{aw}$</td>
<td>-4 to 3</td>
</tr>
<tr>
<td>$\log K_{ow}$</td>
<td>-3 to 10</td>
</tr>
<tr>
<td>Half-life in air</td>
<td>24 to 168 hours (1 to 7 days)</td>
</tr>
<tr>
<td>Half-life in water</td>
<td>960 to 4,320 hours (40 to 180 days)</td>
</tr>
<tr>
<td>Half-life in soil</td>
<td>4,320 to 1,000,000 hours (180 to 41,667 days)</td>
</tr>
</tbody>
</table>

Notes: 1) $K_{aw}$ = air-water partition coefficient.  
2) $K_{ow}$ = octanol-water partition coefficient.

The effects of varying the model input data within these ranges on four endpoints from the model were considered. The endpoints considered were the overall TE, the overall CTD, the TE resulting from release to water and the CTD resulting from release to water. The overall (i.e. highest) TE and CTD results in all cases reflected values calculated for the release to air. The TE and CTD from release to water are the values calculated for that specific release route. Full details of the modelling carried out for this report are given in the Appendix.

When considering the overall CTD, the range of values obtained was 448 km to 3,481 km. The overall CTD depended mainly on the assumed half-life in air. The overall CTD was relatively independent of the assumed half-life in water or soil. The $\log K_{ow}$ had little effect on the overall CTD up to a $\log K_{ow}$ of around 6-7; above this there was an increase in the overall CTD with $\log K_{ow}$ when the $\log K_{aw}$ was around 0 or below. This increase became more marked as the $\log K_{aw}$ decreased.

The overall TE calculated was in the range 0.00014 to 12.6% (out of a possible maximum of 100%). Similar to the overall CTD, the overall TE depended mainly on the assumed half-life in air and was relatively independent of the assumed half-life in water or soil. The overall TE was very low for $\log K_{ow}$ values of around 2 above (<0.0017%) and increased as the $\log K_{aw}$ decreased. The overall TE was relatively independent of $\log K_{ow}$ up to $\log K_{ow}$ of around 6-7, after which the overall TE increased with increasing $\log K_{ow}$.

These results for the overall TE are consistent with transport via the air, where the CTD and TE is governed by volatilisation to the atmosphere and degradation in air. Substances with high $\log K_{aw}$ values have a low potential for deposition on solid media, and hence have a low TE.
This suggests that high water solubility alone may not be sufficient as a criterion for assessing mobility in the environment and suggests that the $K_{aw}$ may also be a relevant consideration.

When the CTD and TE for emissions to water are considered, a slightly different pattern emerges. The CTD was in the range 62 to 392 km. For a given log $K_{aw}$ value the CTD for emissions to water was relatively constant up to a log $K_{ow}$ of around 5, and then decreased slightly with increasing log $K_{ow}$ up to log $K_{ow}$ of around 9. The CTD was predicted to increase with increasing half-life in water. The CTD was relatively insensitive to the log $K_{aw}$ in the range -1 to 3 but increased as the log $K_{aw}$ decreased below the range. The assumed half-life in air had little impact on the CTD estimated over the range studied.

The TE for emissions to water followed a similar pattern to the CTD for emissions to water. Again, the TE increased as the assumed half-life in water increased. The TE values were in the general range $1\times10^{-10}$% to 0.11% and showed a negative correlation with the log $K_{aw}$, tending to increase as the log $K_{aw}$ decreased. For log $K_{aw}$ values of 0 and above the TE calculated was very low (<<0.001%). The TE was also found to be dependent upon the assumed half-life in air.

Taken overall, these results are suggestive that the mobility in the water phase is governed mainly by the persistence in the water phase, and also the transfer from the water phase to the air phase. Thus, for a substance to be highly mobile in the water phase it needs to have a combination of persistence in the water phase, a low to moderate log $K_{ow}$ value and a low air-water partition coefficient. This suggests that the log $K_{aw}$ may be a more relevant parameter to consider than the water solubility alone. For substances with relatively high air-water partition coefficients, mobility in the environment is predicted to be governed mainly by the persistence in air rather than the persistence in water.

In order to investigate the effect of a low log $K_{aw}$ on the mobility, we have carried out further runs of the OECD Screening Tool. Full details of the modelling carried out for this report are given in the Appendix.

The main findings are summarised below.

**For emission to water**

- Predictions of TE, CTD and Pov are effectively independent of the log $K_{ow}$ up to a log $K_{ow}$ of around 6.
- The overall TE is effectively independent of the assumed half-life in water over the range tests. The overall TE for substances with log $K_{ow}$ of 5 or below shows a maximum at a log $K_{aw}$ of around -6. The overall TE reflects transport mainly via the air and is governed more by the persistence in air than the persistence in water in these simulations.
- For substances with log $K_{ow}$ values of 5 or below, the overall CTD is effectively independent of the log $K_{ow}$ values for log $K_{aw}$ values between 0 and around -3, but below this log $K_{aw}$ range the overall CTD shows an increasing trend with the assumed half-life in water. This is consistent with overall CTD for substances with log $K_{aw}$ down to around -3 being governed mainly by transport via the atmosphere but at lower log $K_{aw}$ values the overall CTD is increasingly governed by transport via the water phase.
The water TE for substances with log $K_{ow}$ of 5 or below shows a maximum at a log $K_{aw}$ of around -3 and, in contrast to the overall TE, the water TE increases as the half-life in water increases. The maximum at a log $K_{aw}$ of -3 is likely to reflect two competing processes: a) the potential for volatilisation from water increasing as the log $K_{aw}$ increases, and b) the potential for re-deposition increases as the log $K_{aw}$ decreases. The dependence on the half-life in water is interpreted in terms of a higher build up in the water phase for more persistent substances, resulting in a higher “pool” of substance for volatilisation.

For substances with log $K_{ow}$ values below around 6, the water CTD is relatively independent of the assumed half-life in water for substances with log $K_{aw}$ values in the range 0 to -3. Below this log $K_{aw}$ range the water CTD for substances with log $K_{ow}$ values <6 shows an increasing trend with increasing half-life in water, particularly when the half-life is longer than 3,840 hours (160 days). Again, this is consistent with transport mainly via the air for substances with log $K_{aw}$ of -3 and above, and for substances with log $K_{aw}$ transport via water becomes increasingly important.

For substances with log $K_{ow}$ values <6, the water Pov is relatively independent of the log $K_{ow}$ value for log $K_{aw}$ values down to around -3, and then increases with decreasing log $K_{aw}$ value at or below this value. This increase in the water Pov becomes more marked as the assumed half-life in water increases above 3,840 hours (160 days). Again, this is consistent with transport mainly via the air for substances with log $K_{aw}$ of -3 and above, and for substances with lower log $K_{aw}$ transport via water becomes increasingly important.

For emission to soil

- Predictions of soil TE and soil Pov are effectively independent of the log $K_{ow}$ up to a log $K_{ow}$ of around 2.
- The soil TE shows a maximum at a log $K_{aw}$ of around -3 and the soil TE increases as the half-life in soil increases. Similar to the case with water, the maximum at a log $K_{aw}$ of -3 is likely to reflect two competing processes: a) the potential for volatilisation from soil increasing as the log $K_{aw}$ increases, and b) the potential for re-deposition increases as the log $K_{aw}$ decreases. The dependence on the half-life in soil is interpreted in terms of a higher build up in the soil phase for more persistent substances, resulting in a higher “pool” of substance for volatilisation.
- For substances with a log $K_{ow}$ of 3 or below and with a log $K_{aw}$ value of -2 and above, the soil Pov is effectively independent of the half-life in soil. At higher log $K_{ow}$ values or lower log $K_{aw}$ values the soil, Pov becomes increasingly dependent on the half-life in soil. This is again consistent with volatilisation from soil for substances with lower log $K_{ow}$ values and higher log $K_{aw}$ values, with this becoming less prevalent as the log $K_{ow}$ value increases and/or the log $K_{aw}$ value decreases.

The modelling work carried out suggests that mobility and persistence should be considered together. Transport via water and air are both important processes and, overall, based on our modelling work, it can be concluded that for substances with log $K_{aw}$ values above -3, the mobility in terms of long-range transport is governed mainly by transport via the air and so the mobility is dependent mainly on the persistence in the atmosphere rather than persistence in water or soil. For substances with log $K_{aw}$ values of -3 or below, the persistence in water or soil becomes increasing important to the mobility, and this becomes increasingly marked as the half-life in water or soil exceeds around 180 days.
3.2 Discussion

Our modelling work suggests that mobility and persistence should be considered together.

The OECD POV and LRTP Screening Tool (OECD, 2009) gives “boundary” values of Pov = 195 days, CTD = 5,097 km and TE = 2.248% which define the boundary between substances with a high long-range transport potential and those with a low long-range transport potential. These values are based on model results for ten reference substances including six substances that are known to be POPs or likely to have characteristics of POPs, and four substances with relatively short environmental half-lives and little or no occurrence in remote regions. The boundary values can be used as reference points for screening other chemicals. Modelled values based on mobility and persistence criteria could, therefore, be considered against these boundary values.

The potential for transport via water or air is clearly related to the half-life of a substance in each of those media respectively. Mobility in the water phase is governed in part by the potential to transfer to other phases, for example adsorption onto particulates, volatilisation into air, and also the degradation half-life in these phases. Water solubility of a substance itself only plays an indirect role in the mobility i.e. water solubility limits the ultimate concentration of a substance that can be achieved in the water phase in the environment. The transport and partitioning between different phases (e.g. water to soil, water to air) depend more upon the partition coefficient for these processes rather than the water solubility itself. Although the magnitude of these partition coefficients may be related to the water solubility (for example the air-water partition coefficient), using water solubility alone as a criterion for a mobile substance is not appropriate. This is reflected partly in the criteria proposed by UBA for drinking water, in that it requires a relatively high water solubility (≥0.15 mg/l) and a relatively low log Koc (≤4) or log Kow (≤4) to trigger “mobile”. This may be appropriate when considering protection of drinking water sources but when protecting more remote regions, such as is the aim of the Stockholm Convention, this may not necessarily be appropriate for the following reasons.

- Transport of persistent substances to more remote regions can occur over very long timescales. At these timescales even slow transport processes, such as transport of particulate matter in water by ocean currents could conceivably occur. Thus, even if a substance has a relatively low water solubility and a relatively high log Koc (so that it would not meet the criteria proposed by UBA) this does not fully preclude that the substance could be transported long distances over extended periods of time if the substance is sufficiently persistent. Here persistence needs to be seen in relation to the timeframe of the transport process.
- Volatilisation to air can occur from water and soil. This is greatest for substances with the highest air-water partition coefficients but can still be significant when considering extended distances and timescales for substances with relatively low air water partition coefficients.

9 The POP reference substances are polychlorinated biphenyls (PCB 28, 101 and 180), hexachlorobenzene, α-hexachlorocyclohexane and carbon tetrachloride.
10 The substances are p-cresol, atrazine, biphenyl and aldrin.
11 For example, the theoretical ultimate concentration in the water phase that can be achieved is limited by the water solubility of the substance.
Although for many substances the air compartment can act as a sink for the chemical, transport via air may still be of concern if the substances are potentially persistent in air and have the potential to accumulate in air-breathing organisms. The octanol-air partition coefficient ($K_{oa}$) is a parameter that can be used to indicate the potential for a substance to bioaccumulate in air-breathing organisms (ECHA, 2017). ECHA (2017) suggests that neutral organic substances which are non-biotransformed and efficiently absorbed have the potential to biomagnify in air-breathing organisms if the substance has a $\log K_{oa} \geq 5$ and a $\log K_{ow} \geq 2$. Substances with $\log K_{ow} < 2$ are eliminated rapidly by urinary excretion and so do not biomagnify even if their $\log K_{oa}$ is $\geq 5$.

The $K_{oa}$ can be estimated from the $K_{aw}$ and the $K_{ow}$ using the following relationship:

$$K_{oa} = \frac{K_{ow}}{K_{aw}} \text{ or}$$

$$\log K_{oa} = \log K_{ow} - \log K_{aw}$$

The graph below (Figure 1) indicates the variation of $\log K_{oa}$ with $\log K_{ow}$ for a given value of $\log K_{aw}$ based on this equation. It shows that for substances with a $\log K_{aw}$ of 1 or above, the $\log K_{oa}$ is $\geq 5$ only when the $\log K_{ow}$ is 6 or above. This is important because, as discussed above, in relation to the possible mobility criteria, the substances with high $\log K_{aw}$ values (above $\log K_{aw}$ of 0) are those that are predicted to be mobile (or to transport) mainly via rapid volatilisation to the air. The transport potential for these substances is therefore related to the atmospheric degradation and, importantly, the substances are not likely to be bioaccumulative until the $\log K_{ow}$ reaches high levels ($\log K_{ow}$ of 6 or greater).

For substances with $\log K_{aw}$ of 0 or lower, the $\log K_{oa}$ is $\geq 5$ only when the $\log K_{ow}$ is $\leq 5$. The $\log K_{ow}$ at which the $\log K_{oa}$ is $\geq 5$ decreases as the $\log K_{aw}$ decreases such that at a $\log K_{aw}$ of -7, the $\log K_{oa} = 5$ at a $\log K_{ow}$ of -2. This indicates that within the range of properties where the mobility criteria may be relevant, the potential for bioaccumulation in air-breathing species
increases as the log $K_{aw}$ decreases provided the log $K_{ow}$ is $\geq 2$. For substances with a log $K_{ow}$ <2, based on ECHA (2017), no potential for bioaccumulation would be expected regardless of the log $K_{oa}$ as the substances are expected to be rapidly excreted via urine even if exposure occurred.

The modelling carried out uses the log $K_{ow}$ as a measure of potential to adsorb to organic matter. In general, as the log $K_{ow}$ increases, the log $K_{oc}$ would also be expected to increase. However, there are exceptions to this, for example the log $K_{ow}$ is not relevant for metals, and there are some types of organic chemicals for which the log $K_{ow}$ does not adequately describe their adsorption behaviour. Therefore, in line with the UBA (2017) proposal, it is relevant to also include the log $K_{oc}$ in any criteria as an alternative to the log $K_{ow}$.

Taking all of these considerations into account, this tends to suggest that the following main areas for criteria to support a conclusion that long range transport may be of concern in relation to mobility of POPs.

- **Persistent substances with relatively high log $K_{ow}$ values (log $K_{ow}$ >5) or BCF values >5,000 l/kg.** The substances in this group would include the classical POPs captured by the existing Annex D criteria. This group therefore not considered further in this report.

- **Mobile Group 1.** Persistent substances with log $K_{ow}$ <5 or log $K_{oc}$ < 5 with log $K_{aw}$ >0. These will tend to transport via the atmosphere and so persistence in air is important. Re-deposition into surface media is not significant and bioaccumulation potential in air breathing organisms is not significant.

- **Mobile Group 2.** Persistent substances with log $K_{ow}$ <5 or log $K_{oc}$ <5 with log $K_{aw}$ in the range 0 to -3. These will tend to transport via both water and air, and re-deposition into surface media may be significant. Substances in this group with higher log $K_{ow}$ or log $K_{oc}$ values may be transported partly in the particulate phase in water and/or air.

- **Mobile Group 3.** Persistent substances with log $K_{ow}$ <5 or log $K_{oc}$ <5 with log $K_{aw}$ in the range <3. These will tend to transport mainly via water. Substances in this group with higher log $K_{ow}$ or log $K_{oc}$ values may be transported partly in the particulate phase in water.

Mobile Groups 1 - 3 could form the basis of additional considerations under point (cii) of the Annex D criteria (see Section 1.1) and are the focus of the rest of this report.

4. **How do mobility concerns relate to bioaccumulation concerns?**

The following Sections consider how mobility-based parameters can be viewed alongside bioaccumulation-based parameters.
4.1 Consideration of appropriate timescales

When considering mobility-based concerns it is important that they are framed within an appropriate time scale. It is important to consider that both transport of mobile substances and accumulation in environmental media, be that biota, water, sediment, soil etc., are all time-dependent processes that depend on the rate of input (or uptake) and rate of removal. Assuming a continuous release rate, the ultimate “steady-state” concentration reached in a given environmental compartment is a balance of these parameters.

We have exemplified this by considering a very simplistic system whereby a substance is continuously input into an environmental box (e.g. water). Removal processes (e.g. degradation or other removal process) operate in the box. This simple system can be written in terms of the following kinetic equations.

Rate of input into water = x kg/day.
Rate of degradation in water = $k_{deg} \times [\text{Conc}_{\text{water}}]$

Where $k_{deg}$ = first order degradation rate constant (which is equivalent to \ln 2/half-life for (pseudo-) first order processes).

$[\text{Conc}_{\text{water}}] =$ concentration in water.

The rate of change in concentration in time can then be determined as:

$$\frac{d[\text{Conc}_{\text{water}}]}{dt} = \frac{x}{V} - k_{deg} \times [\text{Conc}_{\text{water}}]$$

Where $V =$ volume of water.

The solution to this rate equation is:

$$[\text{Conc}_{\text{water}}] = \frac{x \times (1 - e^{-k_{deg} \times t})}{k_{deg}}$$

Steady state in such a system occurs when both the rate of input into water is equal to the rate of removal from water. The effect of half-life in such a system is shown in Figure 2. As can be seen, for a given input rate both the expected steady state concentration and the expected time to reach steady state increase as the assumed half-life increases. Although this example is based on water as the transport compartment, the general findings are also relevant for other compartments (e.g. sediment or soil) from which accumulation or exposure to organisms could occur. The concentration at steady state is higher if the half-life is higher.
Figure 2  Effect of half-life on steady-state concentrations in a basic box model.

![Graph showing effect of half-life on steady-state concentrations](image)

The results show that substances that have a low bioaccumulation potential could potentially reach similar levels in biota to substances that are known to bioaccumulate, provided that they are sufficiently persistent in the environment. This crucial point is exemplified below.

Consider a substance that has a half-life in water of 60 days and a BCF value of 5,000 l/kg. Using an extension of the one box model above, we have calculated the nominal concentration in biota by adding in a second box for biota. The relevant rate equations are shown below.

\[
\begin{align*}
\text{Rate of input into water} &= x \text{ kg/day}. \\
\text{Rate of degradation in water} &= k_{\text{deg}} \times [\text{Conc}_{\text{water}}] \\
\text{Rate of uptake into biota} &= k_{\text{uptake}} \times [\text{Conc}_{\text{water}}] \\
\text{Rate of depuration from biota} &= k_{\text{dep}} \times [\text{Conc}_{\text{fish}}]
\end{align*}
\]

Where \( k_{\text{deg}} \) = first order degradation rate constant (which is equivalent to \( \ln 2/\text{half-life} \) for first order processes). 
\( [\text{Conc}_{\text{water}}] \) = concentration in water. 
\( k_{\text{uptake}} \) = uptake rate constant from water into biota. 
\( k_{\text{dep}} \) = depuration rate constant from biota.

In order to simplify the model, we have assumed that the uptake into biota does not significantly affect the concentration in water, and the depuration processes from biota do not lead to significant re-release of the substance to water, as would be the case for a substance that is rapidly metabolised.

Under these conditions, the concentration in biota at any time can be estimated from the concentration in water using the following equation\(^{12}\).

---

\(^{12}\) In order to implement this in the spreadsheet model, the daily increase (or decrease) in the concentration in fish is calculated, which is then added to the concentration in fish from the previous day.
\[
[\text{Conc}_{\text{biota}}] = \frac{[\text{Conc}_{\text{water}}] \times k_{\text{uptake}} \times (1 - e^{-k_{\text{dep}} t})}{k_{\text{dep}}}
\]

Where \([\text{Conc}_{\text{water}}]\) is the concentration in water at a given time point, estimated using the one box model outlined above.

Figure 3 shows the expected time-trend for the concentration in biota using our model for a substance that has a constant daily input rate into water, a degradation half-life in water of 60 days, an uptake rate constant into biota from water of 100 \(\text{l kg}^{-1} \text{d}^{-1}\) and a depuration rate constant of 0.02 \(\text{d}^{-1}\) (this is equivalent to a kinetic BCF of 100/0.02 = 5,000 \(\text{l kg}^{-1}\)). Also shown for comparison are substances with the same daily input rate but with a half-life in water of 365 days or 730 days and a BCF of 250 \(\text{l kg}^{-1}\) (assuming an uptake rate constant of 100 \(\text{l kg}^{-1} \text{d}^{-1}\) and depuration rate constant of 0.4 \(\text{d}^{-1}\)) and a half-life in water of 365 days and a BCF of 800 \(\text{l kg}^{-1}\) (assuming an uptake rate constant of 100 \(\text{l kg}^{-1} \text{d}^{-1}\) and depuration rate constant of 0.125 \(\text{d}^{-1}\)). As can be seen, for a given mass emission rate, as the degradation half-life increases the steady state concentration predicted in biota for substances with relatively low BCF values can, over extended periods of time, approach that of a substance that is considered to have a high bioaccumulation potential, and the steady state concentration ultimately reached is a function of both the persistence and BCF.

Figure 3  Time trends to accumulation in biota

It is also informative to consider the time trend in concentration in biota following cessation of emission into the model. For this simulation, we have assumed a constant input rate for 5,000 days and then the input was stopped. The time trends in the concentrations in biota for the same four substances as considered above are shown in Figure 4.

This shows that the decline in the concentration in biota following cessation of emission is dependent, in part, on the persistence of the substance in the exposure media (in this case water). For the example substances, the concentration in biota is predicted to be higher for the two
substances with BCFs of 250 l kg\(^{-1}\) and 800 l kg\(^{-1}\) than for the substance with a BCF of 5,000 l kg\(^{-1}\) for several years following cessation of emission.

**Figure 4** Time trend in decline in biota concentration following cessation of emission

In summary, we can draw the following general conclusions.

- In terms of ultimate concentrations in biota, there is an important dependence on both the persistence in the exposure medium (e.g. water, sediment or soil) and bioaccumulation potential, as well as emission rates. For a given release rate, the longer the persistence of a substance is, the higher the concentrations that could be reached in an exposure medium, and the lower the bioaccumulation potential would need to be to reach a given concentration in biota exposed to that medium.

- Following cessation of emission to the environment, the decline in concentration in biota is governed, in part, by the rate of degradation in the exposure medium, even when the substance itself is rapidly depurated (or metabolised) from biota. Thus, exposure of biota to highly persistent substances can occur for many years following cessation of emission even if they have a relatively low bioaccumulation potential and/or are themselves depurated rapidly from biota.

- It is important to recognise that the persistence of a substance should be related to the same environmental media in which, or through which, the substance is mobile. For example, the fact that a substance may degrade only slowly in surface water has only limited consequences if the substance is rapidly transferred into the air. Similarly, for a substance to be transported from soil into groundwater the persistence in soil is more relevant than the persistence in surface water.

### 4.2 Significance for mobility

In the POPs context it is informative to consider how mobility-based criteria can be seen in relation to bioaccumulation-based criteria. The analysis carried out in Section 4.1 shows that substances with relatively low BCF values can still potentially reach relatively high levels in
the exposure medium (e.g. water) and organisms over extended timescales if they are sufficiently persistent. Although the analysis carried out in Section 4.1 is based on exposure through water, the same general conclusions would also apply to exposure through water and exposure through soil. Thus, there is a clear relationship between the persistence of a substance and its potential to reach high levels in the environment, including biota.

Importantly in the POPs context, for exposure to occur in remote regions, it is necessary for the substance to be considered mobile enough for it to reach remote regions. Again, as shown in Section 3, persistence is again an important consideration when considering long range transport potential. Thus, persistence can be seen as a factor that provides a linkage between mobility of a substance and potential for the substance to reach relatively high levels in the environment (including biota).

The mobility-based criteria proposed by UBA (2017) are broadly based on the premise that if a substance is sufficiently soluble and does not adsorb strongly to sediment or soil it may be present in the water phase if released to the environment. If the substance is then sufficiently persistent in the environment it may then lead to contamination of water sources (including ground water and drinking water) and hence exposure of organisms including humans.

In relation to the POPs criteria, this approach may be an over simplification. For example, when extended timescales are considered, transport may still occur over long distances even for substances that adsorb strongly to sediments and soil. Indeed, many of the already agreed POPs have high log $K_{ow}$ values or log $K_{oc}$ values and it is known that these POPs can be transported over long distances from sources of release. Hence such substances can be considered as ‘mobile’ in the environment in the general sense. Similarly, the analysis carried out in Section 3 (and further developed in Section 5) also suggests that some substances with relatively high log $K_{ow}$ or log $K_{oc}$ values can be considered to be mobile over extended timescales. This suggests that, in the POPs context, it may be necessary to consider wider criteria for mobility rather than limiting the criteria to those that have relatively low log $K_{ow}$ (or log $K_{oc}$ values) and are likely to be present in the water phase.

The interrelationship between the various factors that govern mobility (transport), occurrence in exposure media (such as air, water, sediment and soil) and occurrence in biota, is complex. For example, substances partition between different exposure media based on their physico-chemical properties and may have a different persistence in each of these exposure media. It is important that the persistence is related to the media in which the substance is considered mobile, or through which it is considered mobile. Thus mobility-based considerations are complex. In Section 5, criteria are proposed for the initial identification of substances that could be considered as persistent and mobile within the POPs context. However, these criteria should be considered as a starting point for the initial identification of potential candidate substances. More detailed environmental modelling of the fate, behaviour and transport potential are needed to fully understand the potential for a given substance to transport long-distances and to accumulate in water, sediment, soil and biota in remote regions. Such modelling is beyond the scope of the current report, but simple modelling approaches as outlined in Section 4.1, could potentially provide useful information\textsuperscript{13} that could be considered alongside more complex models in an integrated approach.

\textsuperscript{13} For example, comparative modelling approaches could be used to compare the substance against a known POP.
Evaluation of using mobility of chemicals in the environment to fulfil bioaccumulation criteria of the Stockholm Convention
5. Definition of possible further criteria for mobility-based concerns for POPs

As described in the previous Sections, for POP substances it is not possible to consider mobility concerns without also considering persistence. Indeed, persistence itself may be the most important parameter to consider in relation to the ultimate mobility of a substance in the environment. When considering extended timescales, even substances that are not considered to be highly mobile in themselves may still be transported and build up in remote areas provided that they are sufficiently persistent. For example, substances that adsorb strongly onto sediment and soil could be transported slowly in these media (for example by sedimentation/resuspension processes in sediment or wind-blown dust/soil in the soil) provided that they are sufficiently persistent within the timescales of these processes.

We have identified three possible subgroups of substance properties in Section 3.2 as a possible basis for mobility-based concerns, and these are elaborated further here. In addition, as is evident in Section 4, extreme persistence in itself may also be a concern, and this is also considered further below.

It is important to stress that, in terms of mobility in the environment, the persistence of a substance should relate to the medium in which the substances are considered to be mobile, or through which they are considered to be transported. An integrated modelling approach may therefore need to be considered to allow the most appropriate measure of persistence to be identified, rather than relying on single media studies which may not be relevant for the mobility concern (for example if a substance is transported by, or is mobile in, mainly the surface water phase, the persistence in sediment or soil may not be relevant considerations).

5.1 Mobile Group 1

These substances are persistent substances with log K_{ow} < 5 or log K_{oc} < 5 with log K_{aw} > 0. These will tend to transport via the atmosphere and so persistence in air is more important than persistence in other media. Re-deposition into surface media is not significant and bioaccumulation potential in air breathing organisms is not significant. This group of substances is unlikely to be of concern in relation to POPs and so it is not necessary to define the group further.

5.2 Mobile Group 2

Persistent substances with log K_{ow} < 5 or log K_{oc} < 5 with log K_{aw} in the range 0 to -3. These will tend to transport via both water and air, and re-deposition from air into surface media may be significant. Substances in this group with higher log K_{ow} or log K_{oc} values may be transported partly in the particulate phase in water and/or air.

Comparison of these parameters with the UBA (2017) proposals for M and vM shows that:

a) A higher log K_{ow} (or log K_{oc}) cut-off of < 5 may be needed than those proposed by UBA (2017) (log K_{ow} or log K_{oc} ≤ 4 for M or ≤ 3 for vM).
b) The log $K_{aw}$ may be a more relevant indicator of mobility than the water solubility indicator proposed by UBA (2017). The $K_{aw}$ can be estimated from the ratio of the vapour pressure of the substance and the water solubility of the substance.

It is also important to consider further what is meant by persistence in this context. The current Annex D criteria are based on a half-life in water of >2 months or half-life in soil or sediment >6 months. These criteria are relevant for the traditional POPs that show a high potential for bioaccumulation (e.g. BCF >5,000 l/kg). However as demonstrated in Section 4, much longer time periods may be needed for substances with lower potential for bioaccumulation to reach levels that may be of concern. This suggests that, when mobility concerns are considered, more stringent persistence criteria should be considered.

The experimental demonstration of long persistence is somewhat problematic as many of the available standard test guidelines for biodegradation (e.g. the OECD Test Guidelines) consist of screening tests, which generally have only limited utility in predicting long persistence. The available biodegradation simulation tests guidelines available are generally recommended to be carried out over 60-120 days dependent on the test. This means that it is difficult to determine experimentally long degradation half-lives in water, sediment and soil.

The modelling carried out suggests a half-life of at least 1 year may be a relevant criterion when considering mobility. This also represents a pragmatic limit of what could theoretically be measured in the standard test systems. For example, if <10% degradation was seen in a 60-120 day test, it could reasonably be extrapolated that the likely half-life would be around 1 year or more.

The persistence should be related to the environmental compartment in which the substance is mobile. This will need to be considered case-by-case taking into account the properties of the substance. For example, substances with relatively low log $K_{ow}$ values (e.g. log $K_{ow}$ <3) would be expected to be present mainly in the water phase but for higher log $K_{ow}$ values they may increasingly be present in the sediment or soil phase. It is important to note that transport via the air may also be important for some members of this group and so it is necessary to consider the overall persistence in an integrated manner.

5.3 Mobile Group 3

Persistent substances with log $K_{ow}$ <5 or log $K_{oc}$ <5 with log $K_{aw}$ in the range < -3. These will tend to transport mainly via water. Substances in this group with higher log $K_{ow}$ values or log $K_{oc}$ values may be transported partly in the particulate phase in water.

Again, in relation to persistence, it would be appropriate to consider a longer half-life than defined by Annex D. As above, a pragmatic minimum half-life of at least 1 year would appear to be appropriate. The persistence should be related to the environmental compartment in which the substance is considered to be mobile. As for mobile group 2, this will need to be considered case-by-case taking into account the properties of the substance.

---

14 For example, the recommended test durations for the OECD Test Guidelines are: 60 days (OECD 306: Biodegradation in Seawater); 120 days (OECD 307: Aerobic and anaerobic transformation in soil); 100 days (OECD 308: Aerobic and anaerobic transformation in aquatic sediment); and 60 days (OECD 309: Aerobic mineralisation in surface water – Simulation biodegradation test).
5.4 Extreme persistence group

This group would consist of substances which have a low bioaccumulation potential (e.g. a BCF <<5,000 l/kg) but which show extreme persistence. This would include both mobile substances and substances that would not be expected to be “mobile” in the sense that they would tend to adsorb strongly onto soil, sediment etc. but their extreme persistence means that, over extended timescales, slow transport could still occur (for example by suspension – redeposition processes or wind-blown dust etc.)

Clearly for these substances, the persistence should be significantly longer than the current Annex D criteria and should be judged in terms of persistence over many years. This would have to be considered on a case-by-case basis.

5.5 Should toxicity also be considered alongside mobility?

The mobility-based considerations identified in Sections 5.1 to 5.4 are suggested as possibilities to be considered in relation to criterion c) ii of Annex D in relation to bioaccumulation. This clause also suggests that high toxicity or ecotoxicity can be considered as evidence. In addition, criterion e) of Annex D also relates to adverse effects to human health or the environment, toxicity or ecotoxicity. It is therefore relevant to consider whether the mobility considerations should also consider toxicity/ecotoxicity.

In terms of the Annex D criteria, criterion e) does not specify specific criteria for determining adverse effects or toxicity/ecotoxicity. The UBA (2017) proposal for PMT gives the following criteria for identifying a substance as toxic (T).

A substance fulfils the toxicity criterion (T) if (UBA, 2017):

a) the long-term no-observed effect concentration (NOEC) or EC10 for marine or freshwater organisms is less than 0.01 mg/l; or
b) the substance meets the criteria for classification as carcinogenic (category 1A, 1B or 2), germ cell mutagenic (category 1A, 1B or 2), or toxic for reproduction (category 1A, 1B, or 2) according to Regulation EC No 1272/2008; or
c) there is other evidence of chronic toxicity, as identified by the substance meeting the criteria for classification: specific target organ toxicity after repeated exposure (STOT RE category 1 or 2) according to Regulation EC No 1272/2008; or
d) the substance meets the criteria for classification as “additional category for effects on or via lactation”, according to Regulation EC No 1272/2008; or
e) the Derived-No-Adverse-Effect-Level (DNEL) is ≤9 μg/kg/d (oral, long term, general population); or
f) the substance acts as an endocrine disruptor in humans and/or wildlife species according to the WHO/IPCS definition of an endocrine disruptor.

These would appear to be relevant criteria for identifying the hazards associated with a substance. Given that one of the main concerns over persistent and mobile substances is that they could build up over time in the environment to levels that may eventually cause effects, it is relevant to take a hazard-based approach to their identification as the timescales involved before levels of concern may be reached may be extremely long (so it may not be possible to
demonstrate that at the current time harm is occurring) and may take a long time to reverse (harm could occur in the future and would be difficult to rectify).

It would therefore be relevant to consider the toxicity alongside mobility for substances in the mobile groups 2 and 3.

For the extreme persistent group, the lack of toxicity in standard tests does not necessarily mean that they have no potential to cause harm over extended timescales. This introduces uncertainty over whether or not effects could occur as a result of prolonged exposure to the substance. Therefore for this group it is suggested that toxicity itself may not always be a relevant criterion in relation to Annex D c)ii (see Section 1.1). This would need to be considered case-by-case.

In summary, the following combinations are suggested in relation to Annex D c)ii.

- **Mobile, Persistent and Toxic (PMT) substances** with log \( K_{ow} < 5 \) or log \( K_{oc} < 5 \) with log \( K_{aw} \) in the range 0 to -3.
  - The persistence should be related to the environmental compartment in which, or through which, the substance is considered to be mobile, and the half-life should be demonstrably >1 year. This will need to be considered case-by-case taking into account the properties of the substance. It is important to note that transport via the air may also be important for some members of this group and so it is necessary to consider the overall persistence in an integrated manner.

- **Persistent, Mobile and Toxic (PMT) substances** with log \( K_{ow} < 5 \) or log \( K_{oc} < 5 \) with log \( K_{aw} \) in the range <-3.
  - The persistence should be related to the environmental compartment in which, or through which, the substance is considered to be mobile, and the half-life should be demonstrably >1 year. This will need to be considered case-by-case taking into account the properties of the substance.

- **Extremely persistent substances.** This group would consist of substances which have a low bioaccumulation potential (e.g. a BCF <<5,000 l/kg) but which show extreme persistence in a relevant environmental media (half-life >>1 year). These would need to be considered on a case-by-case basis.

These suggested criteria are based, in part, on the log \( K_{ow} \). As indicated in Section 2, the octanol-water distribution (\( D_{ow} \)) could be used as an alternative, for ionic and dissociating substances. The \( D_{ow} \) at different pH can be estimated from the log \( K_{ow} \) for several groups of substances including organic acids, bases and amphoteric substances (e.g. see Section 2). Where appropriate, the log \( D_{ow} \) can be used in place of the log \( K_{ow} \) in the above criteria.
6. Case studies

6.1 Examples of existing POPs that have a BCF <5000 l/kg

The following sections considers substances that have been identified as POPs but which do not meet the numerical criteria for bioaccumulation based on BCF. The available data for these substances have been compared against the suggested mobility-based screening criteria developed in this report, and those proposed for PMT and vPvM substances by UBA (2017).

Where the OECD POV and LRTP Screening Tool have been used, plots are presented showing the outcome of the modelling. These plots are divided into four regions (see Figure 5) based on the “boundaries” for POP-like behaviour\(^{15}\) for Pov, TE and CTD given in OECD (2009). Substances in the lower left region do not exceed any of these boundaries and are of low concern for long-range transport whereas substances in the top right region exceed both of the boundaries shown on the plot, and this is the region inhabited by “classical” POPs. Substances in the other two regions exceed one of the boundaries shown and show some POP-like tendency.

**Figure 5** Example plot from the OECD POV and LRTP Screening Tool

For most substances, definition of a single degradation half-life in water, sediment and/or soil is problematic as there are many factors that can affect the degradation half-life. Therefore, where appropriate, a range of degradation half-lives have been considered in order to test the screening criteria. Although it is recognised that some of the degradation half-lives assumed may be unrealistic, such an approach is informative to the development of the screening criteria as it allows important trends to be identified that may be relevant to substances other than those considered here.

It should also be noted that the toxicity of the substances has not been considered as part of this analysis as the focus is on the mobility aspects.

\(^{15}\) The boundaries are: Pov=195 days, CTD = 5097 km and TE = 2.248%. 
6.1.1 alpha-Hexachlorocyclohexane (α-HCH)

The relevant physicochemical properties data for alpha-hexachlorocyclohexane (α-HCH) are summarised below (taken from UNEP, 2008).

<table>
<thead>
<tr>
<th>Table 6.1</th>
<th>Properties of α-HCH</th>
</tr>
</thead>
</table>
| CAS Number(s) | 319-84-6 (racemic)  
119911-69-2 ((+) α-HCH)  
119911-70-5 ((−) α-HCH) |
| Molecular weight | 290.83 g/mol |
| Melting point | 432 K |
| Boiling point | 561 K |
| Water solubility | 0.33 mol/m$^3$ at 25°C  
(96 mg/l) |
| Vapour pressure | 0.25 Pa at 25°C |
| Henry’s Law Constant | 0.74 Pa m$^3$/mol at 25°C |
| Log $K_{ow}$ | 3.9 at 25°C |
| Log $K_{aw}$ | -3.52 at 25°C |
| Log $K_{oa}$ | 7.5 at 25°C |
| Persistence | Moderate persistence in soil. Half-lives in Arctic lakes up to 1.4 years. Half-lives in Eastern Arctic Ocean 5-17 years. Half-life in air 115 days. |
| BCF | 1100-2800 l/kg |
| Other bioaccumulation data | BMFs >1 in invertebrates, fish and terrestrial and marine mammals. Most birds show BMFs <1. |
| Long-range transport | Transport by “cold condensation” on a global scale. |
| Reasons for listing under clauses ii) and iii) | BMFs>1 and detection in human tissues, including exposure during critical periods of development. |

Based on these data, the substance would meet the P, M and vP criteria proposed by UBA (2017) but would not meet the criterion for vM. When considered against the suggested screening criteria developed in this report, the substance would fall into the group of substances with a log $K_{aw}$ < -3 and log $K_{ow}$ < 5 with a degradation half-life of the substance in water of >1 year.

In order to investigate the effect on mobility of assumptions over the degradation rate in water and soil, the OECD POV and LRTP Screening Tool was run with variation of the assumed half-life in both water and soil between 960 hours (40 days) and 70,080 hours (8 years). The resulting plots from the Screening Tool are shown in Figure 6).

At the low end of the assumed half-life range in water and soil, the substance is modelled either at the borderline of, or within, the upper left-hand quadrant, but at assumed half-lives in water and soil of 4,320 hours (180 days) and above the substance is modelled in the top right-hand
quadrant indicating POP-like properties. The actual degradation half-life of the substance in water is >1 year.

The model outputs also show that the CTD is dominated by emissions in air. At lower assumed half-lives in water and soil the TE is also dominated by emissions in air. At higher assumed half-lives in water and soil (starting at around 180 days or more for water and 365 days for soil) the TE from emissions in water and emissions in soil start to approach that for air. This suggests that the mobility of this substance in the environment, in terms of long-range transport, is a result of a combination of a relatively long half-life in air and relatively long half-life in water and soil.

Overall, this substance would screen as persistent and mobile using the screening criteria suggested in this report, and the modelling carried out would tend to support that conclusion.

Figure 6 Long-range transport potential of α-HCH

6.1.2 beta-Hexachlorocyclohexane (β-HCH)

The relevant properties data for beta-hexachlorocyclohexane (β-HCH) are summarised below (taken from UNEP, 2007).
### Table 6.2 Properties of β-HCH

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number(s)</td>
<td>319-85-7</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>290.83</td>
</tr>
<tr>
<td>Melting point</td>
<td>314-315 K</td>
</tr>
<tr>
<td>Boiling point</td>
<td>333 K at 67 Pa.</td>
</tr>
<tr>
<td>Water solubility</td>
<td>1.44 mol/m³ at 25°C (419 mg/l)</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>0.053 Pa at 25°C</td>
</tr>
<tr>
<td>Henry’s Law Constant</td>
<td>0.037 Pa m³/mol at 25°C (K_{aw} = 1.49E-5)</td>
</tr>
<tr>
<td>Log K_{ow}</td>
<td>3.9 at 25°C</td>
</tr>
<tr>
<td>Log K_{aw}</td>
<td>-4.84 at 25°C</td>
</tr>
<tr>
<td>Log K_{oa}</td>
<td>8.7 at 25°C</td>
</tr>
<tr>
<td>Persistence</td>
<td>Under favourable conditions, β-HCH is susceptible to biodegradation. Laboratory and field data including a long-term soil study suggest that β-HCH is persistent in soil, especially under low temperatures. Half-life in air estimated as 56 days.</td>
</tr>
<tr>
<td>BCF</td>
<td>BCFs 250–1,500 (whole body dry weight basis)</td>
</tr>
<tr>
<td>Other bioaccumulation data</td>
<td>Field studies in Arctic marine food webs have demonstrated that β-HCH can bioaccumulate in upper trophic levels. Biomagnification factors for β-HCH in marine food webs were mostly in the range of 1–18 (with a maximum value of 280).</td>
</tr>
<tr>
<td>Long-range transport</td>
<td>Long range transport mainly via ocean currents.</td>
</tr>
<tr>
<td>Reasons for listing under clauses ii) and iii)</td>
<td>Bioaccumulates in upper trophic levels and is persistent in investigated species. Detected in breast milk in humans and also in placenta tissues, thus exposing offspring at critical periods of development.</td>
</tr>
</tbody>
</table>

Based on these data, the substance would meet the P, M and potentially the vP criteria proposed by UBA (2017) but would not meet the criterion for vM. When considered against the suggested screening criteria developed in this report, the substance would fall into the group of substances with a log K_{aw} < -3 and log K_{ow} < 5 with a potentially a long (but undefined) degradation half-life of the substance in water or soil.

In order to investigate the effect on mobility of assumptions over the degradation rate in water and soil, the OECD POV and LRTP Screening Tool was run varying the assumed half-life in both water and soil between 960 hours (40 days) and 70,080 hours (8 years). The resulting plots from the Screening Tool are shown in Figure 7.
Similar to the case with α-HCH, at the low end of the assumed half-life range in water and soil, the substance is modelled either at top end of the bottom left-quadrant or within the upper left-hand quadrant. At assumed half-lives in water and soil of 4,320 hours (180 days) and above the substance is modelled in the top right-hand quadrant for the TE and Pov indicating POP-like properties (the CTD and Pov is modelled in the top right hand box only at an assumed half-life in water or soil of 8 years). The actual degradation half-life of the substance in water and soil is not available.

The model outputs show that the TE is dominated by emissions in air in all cases. At lower assumed half-lives in water and sediment the CTD is also dominated by emissions in air, but at higher assumed half-lives in water and sediment (starting at around 365 days or more for water and 2 years for soil) the CTD from emissions in water and emissions in soil start to approach and then exceed that for air. Again, this suggests that the mobility of this substance in the environment, in terms of long-range transport, is a result of a combination of a relatively long half-life in air and relatively long half-life in water and soil. It is interesting to note the differences here between the modelled results for β-HCH compared with those for α-HCH (generally a higher CTD and TE was estimated for α-HCH compared with β-HCH for a given assumed half-life in soil and sediment). These appear to relate mainly to the lower half-life in air for β-HCH (56 days) compared with α-HCH (115 days) again showing the importance of the transport via air to the mobility.

Overall, this substance would screen as persistent and mobile using the screening criteria suggested in this report, and the modelling carried out would tend to support that conclusion.

### 6.1.3 Lindane (γ-HCH)

The relevant properties data for lindane are summarised below (taken from UNEP, 2006b unless otherwise noted).
Table 6.3 Properties of lindane

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number(s)</td>
<td>58-89-9</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>290.83</td>
</tr>
<tr>
<td>Melting point</td>
<td>112.5°C</td>
</tr>
<tr>
<td>Boiling point</td>
<td>323.4°C</td>
</tr>
<tr>
<td>Water solubility</td>
<td>7.3 mg/l (temperature not stated; taken from NTP, 2016)</td>
</tr>
<tr>
<td>Vapour pressure at 20°C</td>
<td>4.2×10^{-3} mmHg at 20°C</td>
</tr>
<tr>
<td>Henry’s Law Constant</td>
<td>3.5×10^{-6} atm m^3/mol (temperature not stated) K_{aw} = 1.43×10^{-4}</td>
</tr>
<tr>
<td>Log K_{ow}</td>
<td>3.2-3.7 (temperature not stated; taken from WHO, 1991)</td>
</tr>
<tr>
<td>log K_{aw}</td>
<td>-3.84 (temperature not stated)</td>
</tr>
<tr>
<td>Log K_{oa}</td>
<td>7.5 (estimated from the log K_{ow} and log K_{aw})</td>
</tr>
<tr>
<td>Persistence</td>
<td>Half-life in air, water and soil are 2.3 days, 3-300 days and up to 2 to 3 years respectively.</td>
</tr>
<tr>
<td>BCF</td>
<td>10 to 4220 (laboratory conditions); 10 to 2600 (field conditions)</td>
</tr>
<tr>
<td>Other bioaccumulation data</td>
<td>Reported in seabirds, fish and mammals in the Arctic.</td>
</tr>
<tr>
<td>Long-range transport</td>
<td>Accumulates in colder climates of the world. Found in all environmental compartments and levels in air, water, soil, sediment, aquatic and terrestrial organisms have been found worldwide.</td>
</tr>
<tr>
<td>Reasons for listing under clauses ii) and iii)</td>
<td>High toxicity (NOAEL as low as 0.3 mg/kg body weight/day) and ecotoxicity (NOEC &lt;1 µg/l) and reported in seabirds, fish and mammals in the Arctic</td>
</tr>
</tbody>
</table>

Similar to both α-HCH and β-HCH, lindane would meet the P, M and the vP criteria proposed by UBA (2017) but would not meet the criterion for vM. When considered against the suggested screening criteria developed in this report, the substance would fall into the group of substances with a log K_{aw} < -3 and log K_{ow} < 5 with a degradation half-life of the substance in water of up to 1 year and up to 2-4 years in soil.

In order to investigate the effect on mobility of assumptions over the degradation rate in water and soil, the OECD POV and LRTP Screening Tool was run varying the assumed half-life in both water and soil between 960 hours (40 days) and 70,080 hours (8 years). The resulting plots from the Screening Tool are shown Figure 8.
At the lower end of the assumed half-lives in water and soil, the substance would be modelled to be in the bottom left-quadrant indicating the substance would be unlikely to exhibit POP-like properties. As the assumed half-life in water and soil is increased to more realistic values (half-life of 180 days or more), the substance is predicted to show increasingly POP-like properties.

Similar to β-HCH, the model outputs show that the TE is dominated by emissions in air in all cases. At lower assumed half-lives in water and sediment the CTD is also dominated by emissions in air, but at higher assumed half-lives in water and sediment (starting at around 365 days or more for water and 2 years for soil) the CTD from emissions in water and emissions in soil start to approach and then exceed that for air. Again, this suggests that the mobility of this substance in the environment, in terms of long-range transport, is a result of a combination of the half-life in air and relatively long half-life in water and soil.

Again, it is interesting to note the differences here between the modelled results for lindane with those for α-HCH and β-HCH (generally a higher CTD and TE was estimated for α-HCH and β-HCH for a given assumed half-life in soil and sediment). These appear to relate mainly to the lower half-life in air for lindane (2.3 days) compared with α-HCH (115 days) and β-HCH (56 days) again showing the importance of the transport via air to the mobility.

Overall, this substance would screen as persistent and mobile using the screening criteria suggested in this report, and the modelling carried out would tend to support that conclusion.

### 6.1.4 Perfluorooctane sulfonate (PFOS)

The relevant properties data for perfluorooctane sulfonate (PFOS) potassium salt are summarised below (taken from UNEP, 2006a unless otherwise indicated).
### Table 6.4 Properties of PFOS

<table>
<thead>
<tr>
<th>Property</th>
<th>Detail</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number(s)</td>
<td>1763-23-1 (peflurooctane sulfonic acid)</td>
</tr>
<tr>
<td></td>
<td>2795-39-3 (PFOS potassium salt)</td>
</tr>
<tr>
<td></td>
<td>70225-14-8 (diethanolamine salt)</td>
</tr>
<tr>
<td></td>
<td>29081-56-9 (ammonium salt)</td>
</tr>
<tr>
<td></td>
<td>29457-72-5 (lithium salt)</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>538 g/mol (PFOS potassium salt)</td>
</tr>
<tr>
<td>Melting point</td>
<td>&gt;400°C (PFOS potassium salt)</td>
</tr>
<tr>
<td>Boiling point</td>
<td>No measurable (PFOS potassium salt)</td>
</tr>
<tr>
<td>Water solubility at 20°C</td>
<td>519 mg/l</td>
</tr>
<tr>
<td></td>
<td>680 mg/l (PFOS potassium salt)</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>3.31×10⁻⁴ Pa (temperature not stated; PFOS potassium salt)</td>
</tr>
<tr>
<td>Henry’s Law Constant</td>
<td>3.09×10⁻⁹ atm m³/mol (temperature not stated; PFOS potassium salt)</td>
</tr>
<tr>
<td>Log $K_{ow}$</td>
<td>Not measurable (PFOS potassium salt)</td>
</tr>
<tr>
<td></td>
<td>$Log K_{oc} = 2.57^a$</td>
</tr>
<tr>
<td>Log $K_{aw}$</td>
<td>&lt;−5.7 (temperature not stated; PFOS potassium salt)</td>
</tr>
<tr>
<td></td>
<td>−6.9 (estimated here from the Henry’s law constant above assuming a temperature of 25°C)</td>
</tr>
<tr>
<td>Log $K_{oa}$</td>
<td>No data (PFOS potassium salt)</td>
</tr>
<tr>
<td>Persistence</td>
<td>Extremely persistent – it does not hydrolyse, photolys or biodegrade in any environmental condition tested. Half-life in air 114 days.</td>
</tr>
<tr>
<td>BCF</td>
<td>Up to around 2800 l/kg</td>
</tr>
<tr>
<td>Other bioaccumulation data</td>
<td>Accumulates by binding to proteins. Monitoring data show substantial bioaccumulation and biomagnification in top predators.</td>
</tr>
<tr>
<td>Long-range transport</td>
<td>Assumed to be transported in the atmosphere predominantly bound to particles. Atmospheric transport of PFOS precursors is likely.</td>
</tr>
<tr>
<td>Reasons for listing under clauses ii) and iii)</td>
<td>Low elimination rates and high toxicity in mammals (NOAEL of 0.1 mg/kg body weight/day), biomagnification.</td>
</tr>
</tbody>
</table>

Note: The log $K_{ow}$ is not measurable. MST (2015) gives the log $K_{oc}$ for PFOS, potassium salt as 2.57.

Based on these data PFOS would meet the $P$, $M$ and the $vPvM$ criteria proposed by UBA (2017). When considered against the suggested screening criteria developed in this report, the substance would fall into the group of substances with a $log K_{aw} < -3$ and $log K_{oc} < 5$ with a degradation half-life of the substance in water, sediment or soil >1 year.

Although the substance is known to be extremely persistent it is informative to investigate the effect of assumptions of the degradation rate in water and soil on the mobility. Thus, the OECD POV and LRTP Screening Tool was run varying the assumed half-life in both water and soil between 960 hours (40 days) and 70,080 hours (8 years).

The modelling for PFOS is problematical as it is not possible to determine a log $K_{ow}$ value for the substance. For illustrative modelling purposes it has been assumed that the log $K_{oc}$ 2.57 can
be used within the model in place of the log $K_{ow}$. The rationale for this is that the log $K_{ow}$ is usually used as an indicator of the potential for adsorption onto surface media, and the log $K_{oc}$ is also a similar indicator. As discussed earlier, the modelling results are in many cases relatively independent of the log $K_{ow}$ assumed when the log $K_{ow}$ is <5, however, the specific uncertainties inherent in this approach for PFOS are unknown. Therefore, the modelling should be seen as indicative only. The resulting plots from the Screening Tool are shown in Figure 9.

Figure 9   Long-range transport potential of PFOS

As can be seen from the plots the Pov and CTD both increase as the assumed degradation half-life in water and soil increase whereas the TE is not significantly affected by the assumed degradation half-life in water and soil. Thus, the substance is predicted to become increasingly POP-like in terms of CTD as the degradation half-life increases, and the model predicts that the substance would be in the top right-hand quadrant when the half-life in water and soil is 8 years or more.

The model results indicate that TE is governed mainly be emissions in air regardless of the assumed degradation rate in water and soil, whereas the CTD is governed mainly by emissions in water when the degradation half-life in water and soil is 60 days or more.

Overall, this substance would screen as persistent and mobile using the screening criteria suggested in this report, and the modelling carried out would tend to support that conclusion. In addition, the substance would also fall within the extremely persistent substances group.

6.1.5   Perfluorooctanoic acid (PFOA)

Perfluorooctanoic acid (PFOA), its salts and PFOA-related compounds have been proposed for inclusion in Annex A, B and/or C to the Stockholm Convention (UNEP, 2015). The relevant property data summarised below (taken from UNEP, 2016).
Table 6.5  Properties of PFOA (all data relate to pentadecafluorooctanoic acid except where indicated)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number(s)</td>
<td>335-67-1</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>414.07 g/mol</td>
</tr>
<tr>
<td>Melting point</td>
<td>44-56.5°C</td>
</tr>
<tr>
<td>Boiling point</td>
<td>188°C</td>
</tr>
<tr>
<td>Water solubility</td>
<td>9.5 g/l at 25°C, 4.14 g/l at 22°C</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>4.2 Pa at 25°C – value for PFOa, 2.3 Pa at 20°C – value for PFO</td>
</tr>
<tr>
<td>Henry’s Law Constant</td>
<td>No data. Based on a water solubility of 9.5 g/l and a vapour pressure of 4.2 Pa the Henry’s law constant can be estimated as 0.18 Pa m3/mol at 25°C.</td>
</tr>
<tr>
<td>Log K&lt;sub&gt;oc&lt;/sub&gt;</td>
<td>No data. Log K&lt;sub&gt;oc&lt;/sub&gt; = 2.06&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Log K&lt;sub&gt;aw&lt;/sub&gt;</td>
<td>The Henry’s law constant estimated above is equivalent to a K&lt;sub&gt;aw&lt;/sub&gt; of 7.3x10&lt;sup&gt;-5&lt;/sup&gt; (log K&lt;sub&gt;aw&lt;/sub&gt; -4.14).</td>
</tr>
<tr>
<td>Log K&lt;sub&gt;oa&lt;/sub&gt;</td>
<td>No data.</td>
</tr>
<tr>
<td>Persistence</td>
<td>Extremely persistent and does not undergo abiotic or biotic degradation under relevant environmental conditions. Half-life in air estimated to be around 130 days.</td>
</tr>
<tr>
<td>BCF</td>
<td>Low to moderate potential to accumulate in aquatic (water breathing) species.</td>
</tr>
<tr>
<td>Other bioaccumulation data</td>
<td>Evidence for accumulation and biomagnification in air-breathing terrestrial and marine mammals.</td>
</tr>
<tr>
<td>Long-range transport</td>
<td>Found in water, air, sediment and biota from remote locations. Modelling suggests that long-range transport of the substance directly via oceanic circulation, or though transport of precursors followed by formation and deposition of PFOA in remote locations, is plausible.</td>
</tr>
<tr>
<td>Reasons for listing under clauses ii) and iii)</td>
<td>Not yet listed. The substance is persistent, bioaccumulative and toxic to animals including humans. Concluded that PFOA, its salts, and related compounds that degrade to PFOA are likely to lead to significant adverse human health and/or environmental effects as a result of their long-range transport.</td>
</tr>
</tbody>
</table>

Note:  
<sup>a</sup> PFO is the conjugate base of PFOA. The dissociation constant given in UNEP (2016) is 1.5-2.8 with another value given as <1.6. Under most environmental conditions UNEP (2016) indicates that the substance will be present as the PFO anion.  
<sup>b</sup> The log K<sub>oc</sub> is not measurable. MST (2015) gives the log K<sub>oc</sub> for PFOA as 2.06.

Using a similar indicative modelling approach as used for PFOS (using the log K<sub>oc</sub> as a surrogate for log K<sub>aw</sub>), the effects of different assumptions over the degradation half-life in water and soil have been investigated. Thus, the OECD POV and LRTP Screening Tool was run varying the assumed half-life in both water and soil between 960 hours (40 days) and 70,080 hours (8 years). The resulting plots from the Screening Tool are shown in Figure 10.
For PFOA there is an increase in Pov, CTD and TE as the assumed half-life in water and soil increases and the substance appears in the top right-hand sector of the plots when the assumed degradation half-life in water and soil is 180 days or more (based on TE) or 2 years or more (based on CTD).

The TE and CTD is dependent mainly on the emission in air, although the TE and CTD for emissions in water approaches that for air when the assumed degradation half-life in water is around 4 years or more. Again, this shows the importance of considering persistence in air alongside persistence in other media when considering the mobility of a substance over long distances.

Overall, this substance would screen as persistent and mobile using the screening criteria suggested in this report, and the modelling carried out would tend to support that conclusion. Extreme persistence is also likely for this substance and so it would also fall within the group of extremely persistent substances.

### 6.1.6 Perfluorohexane sulphonic acid (PFHxS)

Perfluorohexane sulphonic acid (PFHxS), its salts and PFHxS-related compounds have been proposed for inclusion in Annex A, B and/or C to the Stockholm Convention (UNEP, 2017). The relevant property data summarised below (taken from UNEP, 2017).
Table 6.6  Properties of PFHxS (all data relate to perfluorohexane-1-sulphonic acid)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number(s)</td>
<td>355-46-4</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>400.11 g/mol</td>
</tr>
<tr>
<td>Melting point</td>
<td>272-274°C</td>
</tr>
<tr>
<td>Boiling point</td>
<td>No data</td>
</tr>
<tr>
<td>Water solubility</td>
<td>2.3 g/l at 20-25°C (estimated)</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>58.9 Pa (estimated) at 20°C</td>
</tr>
<tr>
<td>Henry’s Law Constant</td>
<td>No data. Based on a water solubility of 2.3 g/l and a vapour pressure of 58.9 Pa the Henry’s law constant can be estimated as 10.2 Pa m3/mol at 20-25°C.</td>
</tr>
<tr>
<td>Log K_{ow}</td>
<td>5.17 (estimated; the relevance of this prediction is questionable)</td>
</tr>
<tr>
<td>Log K_{oc}</td>
<td>The above Henry’s law constant equivalent to a log Kaw of -2.39.</td>
</tr>
<tr>
<td>Log K_{oa}</td>
<td>7.55 (estimated)</td>
</tr>
<tr>
<td>Persistence</td>
<td>Few data available but read-across from PFOS expected to be extremely persistent. No data on atmospheric half-life. Using the US EPA EPI Suite program, the rate constant for reaction with atmospheric hydroxyl radicals can be estimated as 1.4×10^{-13} cm^3 molecule^{-1} s^{-1}. Assuming an atmospheric hydroxyl radical concentration of 5×10^5 molecule cm^{-3}, the half-life in air can be estimated as 115 days.</td>
</tr>
<tr>
<td>BCF</td>
<td>BCF &lt;&lt; 5,000 l/kg. Experimental data in the range 9.6-133 ion fish.</td>
</tr>
<tr>
<td>Other bioaccumulation data</td>
<td>Expected to bind preferentially to proteins but in fish is expected to be excreted rapidly as a result of its high water solubility. Evidence of biomagnification in field studies from some specific predator-prey studies giving BMFs &gt;1, but TMF studies have generally shown TMFs &lt;1.</td>
</tr>
<tr>
<td>Long-range transport</td>
<td>Log K_{oc} estimated as 1.78. Found in air, soil, sewage sludge and in many species including fish, birds and mammals from the Arctic. Two possible transport mechanisms have been postulated: a) transport of volatile precursors via the atmosphere, degradation by atmospheric oxidation to PFHxS, followed by subsequent wet and dry deposition, and b) direct transport of PFHxS via oceanic currents to the marine environment. Local input from anthropogenic activities may also occur in Arctic regions.</td>
</tr>
<tr>
<td>Reasons for listing under clauses ii) and iii)</td>
<td>Not yet listed. Considered to meet the Annex D screening criteria for persistence, bioaccumulation, long-range transport and adverse effects.</td>
</tr>
</tbody>
</table>

Note:  

a) EPI Suite v4.11.

Similar to PFOS and PFOA, PFHxS would meet the P, M and the vPvM criteria proposed by UBA (2017). When considered against the suggested screening criteria developed in this report, the substance would fall into the group of substances with a log K_{aw} 0 to -3 and log K_{oc} <5 with a degradation half-life of the substance in water, sediment or soil >>1 year.
Using a similar indicative modelling approach as used for PFOS (using the log $K_{oc}$ as a surrogate for log $K_{ow}$), the effects of different assumptions over the degradation half-life in water and soil have been investigated. Thus, the OECD POV and LRTP Screening Tool was run varying the assumed half-life in both water and soil between 960 hours (40 days) and 70,080 hours (8 years). The resulting plots from the Screening Tool are shown below.

**Figure 11** Long-range transport potential of PFHxS

![Plot 1](image1)

![Plot 2](image2)

The CTD, TE and Pov all increase as the assumed degradation half-life in water and soil increase, and the substance appears in the top right-hand sector of the plots (indicating POP-like behaviour) when the half-life in water and soil is 180 days or more.

In all cases the CTD and TE is governed mainly by the emissions in air, although the TE for emissions in water and emissions in soil approach that for air as the half-life in water and soil increases.

Again, this shows the importance of considering persistence in air alongside persistence in other media when considering the mobility of a substance over long distances.

Overall, this substance would screen as persistent and mobile using the screening criteria suggested in this report, and the modelling carried out would tend to support that conclusion. In addition, by read-across to PFOS, the substance may also fall within the extremely persistent substances group.

### 6.2 Other substances that have been indicated as potentially PMT

The proposed mobility-based criteria have also been compared against the data for other substances that have been indicated as potentially of concern based on their persistent, mobile and toxic properties. These are considered in the following Sections.
6.2.1 Methyl tertiary butyl ether (MTBE)

MTBE has been suggested as a potential substance of concern based on its persistence and occurrence in groundwater/drinking water (European Commission, 2017). Relevant property information for MTBE is summarised in the Table below (taken from European Commission, 2002).

Table 6.7 Properties of MTBE

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number(s)</td>
<td>1634-04-4</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>88.15</td>
</tr>
<tr>
<td>Melting point</td>
<td>-108°C</td>
</tr>
<tr>
<td>Boiling point</td>
<td>55.2-55.3°C</td>
</tr>
<tr>
<td>Water solubility</td>
<td>42,000 mg/l at 20°C</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>33,000 Pa at 25°C</td>
</tr>
<tr>
<td></td>
<td>27,000 Pa at 20°C</td>
</tr>
<tr>
<td>Henry’s Law Constant</td>
<td>43.8 Pa m³/mol at 20°C</td>
</tr>
<tr>
<td></td>
<td>53.5 Pa m³/mol at 25°C</td>
</tr>
<tr>
<td>Log Kₐw</td>
<td>-1.67 at 25°C (estimated from the Henry’s law constant)</td>
</tr>
<tr>
<td>Log Kₐw</td>
<td>1.06 at 25°C</td>
</tr>
<tr>
<td>Log Kₒw</td>
<td>2.73 (estimated from the log Kₐw and log Kₐw)</td>
</tr>
<tr>
<td>Persistence</td>
<td>Not readily biodegradable. High degradation rates have been observed in non-standard tests using adapted microorganisms under aerobic conditions, indicating that some microbial species are capable of degrading MTBE, and that MTBE may be inherently biodegradable under certain conditions. Degradation under anaerobic conditions is very slow. Degradation half-life in air is estimated to be 5.65 days.</td>
</tr>
<tr>
<td>BCF</td>
<td>1.5</td>
</tr>
</tbody>
</table>

The European Commission (2017) indicates that the degradation half-life of MTBE in surface waters are dependent upon variables such as current, depth of water and temperature, and gives estimated for the half-life of MTBE in rivers of between 30 minutes and 52 days and in lakes between 10 and 193 days. Degradation in groundwater aquifers was stated to be slow to non-existent under both aerobic and anaerobic conditions.

The substance therefore meets the screening criteria for P and M and vPvM proposed by UBA (2017).

With regards to the screening criteria developed in this report, the log Kₐw for the substance is -1.67 and so the substance falls within the range where transport via air as well as water may be important. There is some uncertainty over the actual degradation half-life of the substance in water, and the available evidence is that it could be below the 1 year threshold suggested as a screening criterion for PMT substances with log Kₒw <5 and log Kₐw in the range 0 to -3 in this report. In order to investigate the effect of assumptions of the degradation rate in water and soil, the OECD POV and LRTP Screening Tool was run varying the assumed half-life in both
water and soil between 960 hours (40 days) and 560,640 hours (64 years). The resulting plots from the Screening Tool are shown in Figure 12.

Regardless of the assumed half-life in water and soil, the substance is modelled in the bottom left quadrant of the plots, indicating that long-range transport of the substance is not of concern for this substance. The transport for this substance is predicted to be predominantly by air, and the assumed half-life in water or sediment has only limited impact on this.

Based on this analysis MTBE would be unlikely to be of concern in a POPs context.

**Figure 12**  
**Long-range transport potential of MTBE**

6.2.2 Substances identified in UBA (2018)

The UBA (2018) study identified a total of 9 substances that were considered to meet the criteria proposed by UBA for PMT and a further 20 substances that were considered to meet the criteria for P and M that also had some indications of toxicity. These substances are summarised in
Table 6.8 Error! Reference source not found. below, along with key property information. The property information was taken from the respective REACH registration dossiers for the substances on the ECHA website\textsuperscript{16}. Where necessary and possible data gaps were filled using estimates from the USEPA EPI Suite\textsuperscript{17}. For two of the substances, no registration dossier was available on the ECHA website and uncertainties over the structure of the substances meant that it was not possible to estimate the missing data. For a further substance, it was not possible to fill the data gaps using the USEPA EPI Suite. Therefore, these substances were excluded from the subsequent analysis carried out here.

\textsuperscript{16} https://www.echa.europa.eu/information-on-chemicals

\textsuperscript{17} The most common data gap was the half-life in air. These were filled by using the estimated hydroxyl radical rate constant assuming an average atmospheric hydroxyl radical concentration of $5 \times 10^5$ molecules/cm$^3$. 
### Table 6.8  Substances identified as PMT or PM with indications of toxicity in the UBA (2018) study

<table>
<thead>
<tr>
<th>Substance/CAS</th>
<th>Molecular weight</th>
<th>$\log K_{aw}$</th>
<th>$\log K_{ow}$</th>
<th>Half-life in air$^a$ (hours)</th>
</tr>
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<tbody>
<tr>
<td>1,2-Dichloroethane 107-06-2</td>
<td>98.96</td>
<td>2.11</td>
<td>1.45</td>
<td>1,750</td>
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<tr>
<td>Tetrachloroethylene 127-18-4</td>
<td>165.83</td>
<td>3.44</td>
<td>2.53</td>
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<td>Trichloroethene 79-01-6</td>
<td>131.39</td>
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<tr>
<td>4-Aminophenol 123-30-8</td>
<td>109.13</td>
<td>-4.05</td>
<td>-0.09</td>
<td>5</td>
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<tr>
<td>1,2,4-Triazole 288-88-0</td>
<td>69.07</td>
<td>-3.57</td>
<td>-0.76</td>
<td>3,851</td>
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<tr>
<td>1,4-Dioxane 123-91-1</td>
<td>88.11</td>
<td>-0.42</td>
<td>-0.42</td>
<td>14</td>
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<td>4-Mesyl-2-nitrotoluene 1671-49-4</td>
<td>215.22</td>
<td>-2.89</td>
<td>0.93</td>
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<tr>
<td>2,6-Dimethylaniline 87-62-7</td>
<td>121.18</td>
<td>-0.53</td>
<td>1.96</td>
<td>2</td>
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<td>2,2,6,6-Tetramethyl-4-oxyperidinoxy 2896-70-0</td>
<td>171.24</td>
<td>-2.98</td>
<td>0.28</td>
<td>6</td>
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<td>1,3,5-Triazine-2,4,6-triamine 108-78-1</td>
<td>108.78</td>
<td>-9.57</td>
<td>-1.22</td>
<td>584</td>
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<tr>
<td>Cyanguanidine 461-58-5</td>
<td>84.08</td>
<td>-5.65</td>
<td>-1.00</td>
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<td>Benzenesulfonic acid, 2,2’-(1,2-ethenediyl)bis[5-[4-[bis(2-hydroxyethyl)amino]-6-(phenylamino)-1,3,5-triazin-2-yl]amino]-, disodium salt 4193-55-9</td>
<td>962.97</td>
<td>No estimate possible</td>
<td>No estimate possible</td>
<td>1</td>
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<td>2-Propanol, 1-chloro-, phosphate (3:1) 13674-84-5</td>
<td>327.57</td>
<td>-3.37</td>
<td>2.68</td>
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<tr>
<td>1,3,5-Triazine-2,4-diamine, 6-phenyl-91-76-9</td>
<td>187.21</td>
<td>-5.03</td>
<td>1.38</td>
<td>105</td>
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<tr>
<td>A mixture of: cis-tetrahydro-2-isobutyl-4-methylpyran-4-ol; trans-tetrahydro-2-isobutyl-4-methylpyran-4-ol 63500-71-0</td>
<td>172.27</td>
<td>-2.14</td>
<td>1.65</td>
<td>8</td>
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<tr>
<td>2,4,7,9-Tetramethyldec-5-yne-4,7-diol 126-86-3</td>
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<td>2.64</td>
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<td>4-Methylmorpholine 4-oxide monohydrate 7529-22-8</td>
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<td>4-Hydroxy-2,2,6,6-tetramethylpiperidinoxy 2226-96-2</td>
<td>172.25</td>
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<td>0.56</td>
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</table>
The evaluation of mobility of chemicals in the environment to fulfil bioaccumulation criteria of the Stockholm Convention

<table>
<thead>
<tr>
<th>Substance/CAS</th>
<th>Molecular weight</th>
<th>log $K_{aw}$</th>
<th>log $K_{ow}$</th>
<th>Half-life in air$^a$ (hours)</th>
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</thead>
<tbody>
<tr>
<td>Sodium 2-[(2-aminoethyl)amino]ethane sulphonate 34730-59-1</td>
<td>190.19</td>
<td>0.01</td>
<td>&lt;-3.1</td>
<td>3</td>
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<td>Dapsone 80-08-0</td>
<td>248.3</td>
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<tr>
<td>Tricarbonylmethylcyclopentadienylmanganese (MMT) 12108-13-3</td>
<td>218.09</td>
<td>2.33</td>
<td>3.4</td>
<td>0.026$^b$</td>
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<td>2,2'-Azobis[2-methylbutyronitrile] 13472-08-7</td>
<td>192.27</td>
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<td>2.07</td>
<td>130</td>
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<td>1-Ethyl-3-methylimidazolium ethylsulfate 342573-75-5</td>
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<td>No estimate possible</td>
<td>No estimate possible</td>
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<td>1-(2,6-bis(4-Tolyl)-1,3-dioxano(5,4-d)-1,3-dioxa-4-yl)ethane-1,2-diol 54686-97-4</td>
<td></td>
<td>No estimate possible</td>
<td>No estimate possible</td>
<td>No estimate possible</td>
</tr>
<tr>
<td>4-Amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide 129909-90-6</td>
<td>241.3</td>
<td>-6.38</td>
<td>1.18</td>
<td>62</td>
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<td>O-Isopropyl ethylthiocarbamate 141-98-0</td>
<td>147.24</td>
<td>1.72</td>
<td>2.3</td>
<td>8</td>
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<tr>
<td>Triethylphosphonoacetate 867-13-0</td>
<td>224.2</td>
<td>-4.45</td>
<td>1.13</td>
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</tr>
<tr>
<td>6-Methyl-1,3,5-triazine-2,4-diyl diamine 542-02-9</td>
<td>125.13</td>
<td>-1.36</td>
<td>-0.88</td>
<td>612</td>
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<tr>
<td>Toluene-2-sulphonamide 88-19-7</td>
<td>171.22</td>
<td>-3.06</td>
<td>0.60</td>
<td>315</td>
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</tbody>
</table>

Note:

a) The half-life in air was estimated from the hydroxyl radical rate constant assuming an atmospheric hydroxyl radical concentration of $5 \times 10^5$ molecules/cm$^3$.

b) The substance degrades rapidly in sunlight with a half-life <1.55 minutes.

The substances with sufficient data were then investigated using the OECD Pov and LRTP Screening Tool. As before, the sensitivity of the modelling to the assumed half-life in water and soil was investigated in the modelling (range of half-lives considered was 960 hours (40 days) to 70,080 (8 years)). The plot below shows that range of range of estimates obtained.
Evaluation of using mobility of chemicals in the environment to fulfil bioaccumulation criteria of the Stockholm Convention

Figure 13  Long-range transport potential of the substances identified by UBA (2018)

Clearly the substances cover a range of transport potential and “POP”-like properties and shows that the criteria proposed in UBA (2017) are not sufficiently selective for identification of mobility-based concerns in relation to POPs.

The substances identified by UBA include six substances with a log $K_{aw} > 0$. As discussed previously these substances are expected to be mobile or transported mainly via the air and are unlikely to re-deposit to surface media in remote regions. Figure 14 shows the long-range transport potential for these substances, predicted using the OECD Pov and LRTP Screening Tool.

Figure 14  Long-range transport potential of the six substances with log $K_{aw} > 0$

As can be seen, all of these substances have a low TE. Three of the substances are predicted to be transported long distances via the air. These are trichloroethene, tetrachloroethylene and 1,2-dichloroethane and all have long half-lives in air. The remaining three substances all appear in the bottom left-hand sector of the plots regardless of the assumed half-life in water or soil.
is consistent with the analysis carried out earlier in this report, which suggested that mobile substances with log \( K_{aw} > 0 \) are of limited concern in relation to POPs.

For the remaining substances, the long-range transport potential, and hence long-range mobility, is a complex combination of the half-life in air and half-life in water and soil.

### 6.3 Discussion of case studies, lessons learned and final suggested screening criteria

The available data for the existing and proposed POPs considered in Section 6.1 show that all of these substances would meet the suggested screening criteria developed for this report.

However, the modelling carried out shows the importance of considering the persistence in air alongside the persistence in other media, and suggests that for some substances with relatively long degradation half-lives in air (of the order of 50 days or more), the suggested persistence cut-off of 1 year for degradation in water and soil may be too long and it may be appropriate to consider a shorter half-life in water or soil of around 180 days.

The modelling carried out for the substances that have been proposed as potentially meeting the PMT or vPvM criteria based on the UBA (2017) criteria has shown that it is appropriate to also consider volatility (in terms of the log \( K_{aw} \)) when mobility over long-ranges is considered rather than specifically occurrence in drinking water sources.

Overall, the analysis suggests that the following screening criteria are relevant for identifying candidate substances for further work in relation to mobility-based concerns within a POPs context.

- **Mobile, Persistent and Toxic (PMT) substances with \( \log K_{ow} < 5 \) or \( \log K_{oc} < 5 \) with \( \log K_{aw} \) in the range 0 to -3.**
  - The persistence should be based on the degradation half-life in water, sediment or soil and be related to the environmental compartment in which, or through which, the substance is considered to be mobile. The half-life in water, sediment or soil should be demonstrably >1 year.
  - It is important to note that transport via the air may also be important for some members of this group and so it is necessary to consider the overall persistence in an integrated manner. When the half-life in air is long (>50 days) it may be appropriate to reduce the half-life in water, sediment or soil to 180 days.

- **Persistent, Mobile and Toxic (PMT) substances with \( \log K_{ow} < 5 \) or \( \log K_{oc} < 5 \) with \( \log K_{aw} \) in the range <-3.**
  - The persistence should be based on the degradation half-life in water, sediment or soil and be related to the environmental compartment in which, or through which, the substance is considered to be mobile. The half-life in water, sediment or soil should be demonstrably >1 year.
  - When the half-life in air is long (>50 days) it may be appropriate to reduce the half-life in water, sediment or soil to 180 days.
• Extremely persistent substances. This group would consist of substances which have a low bioaccumulation potential (e.g. a BCF <<5,000 l/kg) but which show extreme persistence in a relevant environmental media (half-life >>1 year).

It is important to note that mobility-based concerns are a result of a combination of a number of factors and it is difficult to capture all of these factors within simple numerical criteria. Therefore, the screening criteria developed should be seen as the starting point for identifying potential candidates for further evaluation. Proper assessment of mobility based concerns requires understanding of the actual modes of transport and the interaction of the various partitioning and degradation processes that may occur, and needs to be considered on a case-by-case basis by using in-depth modelling and assessment methods. Such assessment approaches are beyond the scope of the current project.

7. Identified concerns over the suggested approaches

Determination of environmental persistence is not straightforward, particularly when half-lives approach the order of years or more. Current test methods are usually carried out over a relatively short timescale.

Other potential issues include:

• Lack of ready biodegradability is not on its own sufficient to equate to persistency.
• The sorption tendency of chemicals may not always relate to the log K\text{ow} (or log D\text{ow}), for example for ionic chemicals, highly polar chemicals, metals etc.
• Monitoring of highly polar persistent and mobile substances presents significant analytical challenges (e.g. see Reemstma et al., 2016).
8. References


NTP (2016). Lindane, hexachlorocyclohexane (technical grade), and other hexachlorocyclohexane isomers. Report on Carcinogens, 14th Edition, National Toxicology Program


UBA (2017). Protecting the sources of our drinking water. A revised proposal for implementing criteria and an assessment procedure to identify Persistent, Mobile and Toxic (PMT) and very Persistent, very Mobile (vPvM) substances registered under REACH. UmweltBundesamt, German Environment Agency, Second, revised edition, October 2017.


Annex I: OECD POV and LRTP Screening Tool Modelling Results

This Annex contains a summary of the results of the modelling that has been carried for this report out using the OECD POV and LRTP Screening Tool (OECD, 2009). We have carried out a number of runs of the OECD Screening Tool in order to explore the properties of chemicals that may support long range transport. This was based around the PMT and vPvM criteria that have been proposed by UBA (2017) and to further explore the importance the environmental half-life and air-water partitioning coefficient in relation to mobility within this modelling system.

Part 1. Properties supporting LRT based around the PMT and vPvM criteria proposed by UBA (2017)

In order to explore the predicted behaviour of substances potentially meeting the PMT and vPvM criteria proposed by UBA (2017) the OECD POV and LRTP Screening Tool was run for a series of hypothetical chemicals by varying the model input data within the following ranges.

- Molecular weight: 200 g/mole (same value used in all model runs)
- Log $K_{aw}^{18}$: -4 to 3
- Log $K_{ow}^{19}$: -3 to 10
- Half-life in air: 24 to 168 hours (1 to 7 days)
- Half-life in water: 960 to 4320 hours (40 to 180 days)
- Half-life in soil: 4,320 to 1,000,000 hours (180 to 41,667 days)

Plots showing how the predicted overall transport efficiency (TE), the overall characteristic travel distance (CTD), the TE resulting from release to water and the CTD resulting from the release to water, and how these predictions vary with the assumed chemical property data are shown below.

In each case the legend in the plot has the following format: Log $K_{aw}$, x hrs, y hrs, z hrs, where log $K_{aw}$ relates to the log $K_{aw}$ value assumed, x is the assumed half-life in air in hours, y is the assumed half-life in water in hours and z is the assumed half-life in soil in hours.

Please note, in some model runs, very similar results were obtained from some combinations of properties assumed and so only one line is shown on the plots. Where this occurs the other combinations referred to in the legend lead to essentially the same results as those shown.

a) Overall TE – effect half-life in air and log $K_{ow}$ for a given log $K_{aw}$

The first series of plots (Figure 15) show how the overall TE varies with the assumed half-life in air and the log $K_{ow}$ for a given log $K_{aw}$ value. For all of these simulations the half-life in water (960 hours) and half-life in soil (1×10^6 hours) were kept constant.

---

18 $K_{aw}$ = air-water partition coefficient.
19 $K_{ow}$ = octanol-water partition coefficient.
The overall TE increases with increasing half-life in air, and also increases as the log $K_{aw}$ decreases within the range studied. The overall TE is effectively independent of the log $K_{aw}$ up to a log $K_{ow}$ of around 6, and then increases with increasing log $K_{ow}$.

Figure 15  Effect of half-life in air and log $K_{ow}$ on the overall TE for a given log $K_{aw}$

These results are consistent with transport occurring mainly via the air. The fact that the transport efficiency increases as the log $K_{aw}$ decreased suggests, that within the range tested, the potential for re-deposition is inversely related to the log $K_{aw}$. Thus, substances with high log $K_{aw}$ values are predicted to essentially remain in the atmosphere (and hence have a low TE) but as the log $K_{aw}$ decreases the potential for deposition back to land or water increases.
b) Overall TE – effect of half-life water and soil and log $K_{ow}$ for a given log $K_{aw}$

The second series of plots show how the overall TE varies with the assumed half-life in water or soil and the log $K_{ow}$ for a given log $K_{aw}$ value. For all of these simulations the half-life in air (48 hours) was kept constant.

**Figure 16** Effect of half-life in water and soil and log $K_{ow}$ on the overall TE for a given log $K_{aw}$

For a given log $K_{aw}$ the overall TE predicted was essentially unaffected by the assumed half-life in water or soil within the range tested. The predicted overall TE was essentially independent of the log $K_{ow}$ value assumed up to a log $K_{ow}$ value of around 6, above which a marked increase in overall TE was predicted with increasing log $K_{ow}$. The overall TE was predicted to increase as the log $K_{aw}$ decreased and the overall TE was <1% for all combinations when the log $K_{aw}$ was 1 or above. Again, these results are consistent with transport occurring mainly via the air and the potential for subsequent re-deposition increasing as the log $K_{aw}$ decreased.
c) Water TE – effect of half-life in air and log $K_{ow}$ for a given log $K_{aw}$

The third series of plots show how the water TE varies with the assumed half-life in air and the log $K_{ow}$ value for a given log $K_{aw}$ value. For all of these simulations the half-life in water (960 hours) and half-life in soil (1×10^6 hours) were kept constant.

**Figure 17** Effect of half-life in air and log $K_{ow}$ on the water TE for a given log $K_{aw}$

Similar to the previous simulations, the transport efficiency was independent of the log $K_{ow}$ up to a log $K_{ow}$ around 6. The TE increased with increasing half-life in air, suggesting that transport was mainly via the atmosphere. The TE initially increased as the log $K_{aw}$ decreased from 3 to around -3 and then decreased again at a log $K_{aw}$ of -4. This latter finding can be interpreted in terms of two competing effects: a) the potential for re-deposition increasing as the log $K_{aw}$ decreases; and b) the potential for volatilisation from water decreasing as the log $K_{aw}$ decreases. Thus, when releases to water are considered there is a “maximum” in the predicted TE at around log $K_{aw}$ of -3.
d) Water TE – effect and half-life in water and soil and log $K_{ow}$ at a given log $K_{aw}$

The fourth series of plots show how the water TE varies with the assumed half-life in water or soil and log $K_{ow}$ at a given log $K_{aw}$ value. For all of these simulations the half-life in air (48 hours) was kept constant.

Figure 18  Effect of log $K_{ow}$ and half-life in water and soil on the water TE for a given log $K_{aw}$

Again, the transport efficiency was independent of the log $K_{ow}$ up to a log $K_{ow}$ around 6. The TE increased with increasing half-life in water, but was independent of the assumed half-life in soil. The TE initially increased as the log $K_{aw}$ decreased from 3 to around -3 and then decreased again at a log $K_{aw}$ of -4. This latter finding can be interpreted in terms of two competing effects: a) the potential for re-deposition increasing as the log $K_{aw}$ decreases; and b) the potential for volatilisation from water decreasing as the log $K_{aw}$ decreases. Thus, when releases to water are considered there is a “maximum” in the predicted TE at around log $K_{aw}$ of -3. The half-life in water is also important to the water TE.
e) Overall CTD– effect of half-life in air and log $K_{ow}$ for a given log $K_{aw}$

The fifth series of plots show how the overall CTD varies with the assumed half-life in air and the log $K_{aw}$ value. For all of these simulations the half-life in water (960 hours) and half-life in soil ($1\times10^6$ hours) were kept constant. Similar to the previous simulations, the overall CTD was independent of the log $K_{ow}$ up to a log $K_{ow}$ of around 6. The overall CTD was dependent on the assumed half-life in air but was effectively independent of the log $K_{aw}$ until the log $K_{aw}$ decreased to -2 or below, after which the overall CTD decreased as the log $K_{aw}$ decreased. Again, this is consistent with transport being mainly via the atmosphere for high and moderate log $K_{aw}$. The decrease in the overall CTD as the log $K_{aw}$ decreases below this range is considered in more detail in Part 2 of the analysis later in this Annex.

**Figure 19** Effect of half-life in air and log $K_{ow}$ on the overall CTD for a given log $K_{aw}$
f) Overall CTD – effect of half-life water and soil and log K\textsubscript{ow} for a given log K\textsubscript{aw}

The sixth series of plots show how the overall CTD varies with the assumed half-life in water or soil and the log K\textsubscript{ow} for a given log K\textsubscript{aw} value. For all of these simulations the half-life in air (48 hours) was kept constant.

As before, the overall CTD was independent of the log K\textsubscript{ow} up to a log K\textsubscript{ow} of around 6, after which the CTD increased, the increase being most marked at log K\textsubscript{aw} values of 0 and below. For a given log K\textsubscript{aw} value the CTD was essentially independent of the assumed half-life in water or soil suggesting that overall CTD was governed mainly by transport via the air. The CTD was not dependent on the log K\textsubscript{aw} assumed at log K\textsubscript{aw} values above -2 but decreased slightly as the log K\textsubscript{aw} decreased below this value. This is considered further in Part 2 of this Annex.

**Figure 20** Effect of half-life in water and soil and log K\textsubscript{ow} on the overall CTD for a given log K\textsubscript{aw}
g) Water CTD – effect of half-life in air and log $K_{ow}$ for a given log $K_{aw}$

The seventh series of plots show how the water CTD varies with the assumed half-life in air and the log $K_{ow}$ for a given log $K_{aw}$ value. For all of these simulations the half-life in water (960 hours) and half-life in soil ($1\times10^6$ hours) were kept constant.

Similar to the previous case, these plots show that the CTD is independent of the log $K_{ow}$ up to a log $K_{ow}$ of 6, above which there is slight decrease in the CTD. The CTD does not depend significantly on the assumed half-life in air over the range studied for log $K_{aw}$ values >-2, but below this value there is a slight increase in the CTD as the half-life in air increases. This is considered further in Part 2 of this Annex.

**Figure 21** Effect of half-life in air and log $K_{ow}$ on the water CTD for a given log $K_{aw}$
h) Water CTD – effect of half-life water and soil and log $K_{ow}$ for a given log $K_{aw}$

The eighth series of plots show how the water TE varies with the assumed half-life in water or soil and the log $K_{ow}$ for a given log $K_{aw}$ value. For all of these simulations the half-life in air (48 hours) was kept constant.

Similar to other simulations, the water CTD is effectively independent of the log $K_{ow}$ up to a log $K_{ow}$ of 6, after which there is a slight decline in the CTD with increasing log $K_{ow}$. The water CTD is clearly dependent on the assumed half-life in water, but is independent of the assumed half-life in soil. The predicted water CTD shows little dependence on the log $K_{aw}$ at log $K_{aw}$ values $> -2$, but increases with decreasing log $K_{aw}$ below this value. This is considered further in Part 2 of this Annex.

Figure 22  Effect of half-life in water and soil and log $K_{ow}$ on the water CTD for a given log $K_{aw}$
Summary of Part 1

The modelling carried out around the proposed UBA PMT criteria reveals several interesting trends.

- The predictions are effectively independent of the log $K_{ow}$ value up to a log $K_{ow}$ of around 6.
- The overall TE and overall CTD reflect mainly transport via air and so the overall TE and overall CTD parameters are generally dependent on the half-life of the substance in air.
- The overall TE estimates suggest that substances with relatively high log $K_{aw}$ values have lower potential for deposition back to land) than substances lower log $K_{aw}$ values. When the log $K_{aw}$ was >0 the overall TE was generally very low.
- There was a “maximum” in the predicted water TE at a log Kaw of around -3 which suggests that the water TE is dependent on two competing factors: a) the potential for volatilisation from water increasing as the log $K_{aw}$ increases; and b) the potential for re-deposition increasing as the log $K_{aw}$ decreases.
- The water TE is dependent on the assumed half-life in water and air, showing an increase with increasing half-life. This suggests of increasing half-life in water leads to increasing concentrations in water which in turn can lead to increasing amounts volatilising to air with subsequent transport. This aspect is considered further in Part 2 of this Annex.
- The water CTD does not depend significantly on the assumed half-life in air over the range studied for log $K_{aw}$ values >-2, but below this value there is a slight increase in the water CTD as the half-life in air increases. The water CTD increases as the assumed half-life in water increases and shows little dependence on the log $K_{aw}$ for log $K_{aw}$ values >-2, but increases with decreasing log $K_{aw}$ below this value. This aspect is considered further in Part 2.

Overall, the analysis carried out around the proposed UBA PMT criteria show that the air-water partition coefficient is an important parameter to consider in relation to the mobility of substances in water. In addition, the simulations are effectively independent of the log $K_{ow}$ value assumed when the log $K_{ow}$ value is <6. For substances with log $K_{aw}$ values >0, the main mode of “mobility” appears to be by volatilisation to the atmosphere followed by transport in the atmosphere. Thus, the mobility of substances with log $K_{aw}$ values >0 is governed mainly by their atmospheric degradation.

For substances with log $K_{aw} <0$ the situation appears to be more complicated and a more detailed investigation of the transport potential and mobility of such chemicals is carried out in Part 2 of this Annex.
Part 2. More detailed investigation of the effects of log $K_{aw}$ and degradation half-life in water

Further runs of the OECD POV and LRTP Screening Tool have been undertaken to investigate the effects of log $K_{aw}$ and degradation half-life of the mobility of chemicals within this modelling framework. The Screening Tool was run by varying the input data within the following ranges.

- **Molecular weight**: 200 g/mole (same value used in all model runs)
- **Log $K_{aw}$**: -7 to 0
- **Log $K_{ow}$**: -3 to 10
- **Half-life in air**: 48 hours (same value used in all model runs)
- **Half-life in water**: 960 to 15,360 hours (40 to 640 days)
- **Half-life in soil**: 1,000,000 hours (41,667 days; same value used in all model runs)

Plots showing the predicted overall transport efficiency (TE), the overall characteristic travel distance (CTD), and the TE, CTD and the overall persistence resulting from release to water (Pov), and how these predictions vary with the assumed chemical property data are shown below.

In each case the legend in the plot has the following format: Log $K_{aw}$, x hrs, where log $K_{aw}$ relates to the log $K_{aw}$ value assumed, x is the assumed half-life in water in hours. In all runs the half-life in air was set to 48 hours and the half-life in soil was set to 1,000,000 hours.

The plots also show the relevant TE, CTD or Pov “boundary” used in the OECD POV and LRTP Screening Tool for identifying substances with POP-like behaviour. If the TE, CTD or Pov calculated for a substance is above this boundary, then the substance shows POP-like behaviour.

Please note, in some model runs, very similar results were obtained from some combinations of properties assumed and so only one line is shown on the plots. Where this occurs, the other combinations referred to in the legend lead to essentially the same results as those shown.

**a) Overall TE – effect half-life in water and log $K_{ow}$ for a given log $K_{aw}$**

The first series of plots show how the overall TE varies with the assumed half-life in water and log $K_{ow}$ value for a given log $K_{aw}$ value. For all of these simulations the half-life in air (48 hours) and half-life in soil ($1 \times 10^6$ hours) were kept constant.
These plots show that the overall TE is independent of the assumed half-life in water over the extended range tested. The overall TE for substances with log $K_{ow}$ of 5 or below does depend on the log $K_{aw}$, with the overall TE initially increasing as the log $K_{aw}$ decreases and then showing the opposite trend, reaching a maximum at a log $K_{aw}$ of around -6 in these simulations. The overall TE is also relatively independent of the log $K_{ow}$ at lower log $K_{ow}$ (<5) but shows an increasing dependence on the log $K_{ow}$ at higher values as the log $K_{aw}$ decreases.

b) Overall TE – effect of log $K_{aw}$ and log $K_{ow}$ for a given half-life in water

The second series of plots show how the overall TE varies with the log $K_{aw}$ and log $K_{ow}$ for a given half-life in water. For all of these simulations the half-life in air (48 hours) and half-life in soil ($1 \times 10^6$ hours) were kept constant. These plots show essentially the same trend as noted in simulation a) above.
c) Water TE – effect of half-life in water and log $K_{ow}$ for a given log $K_{aw}$ value

The third series of plots show how the water TE varies with the assumed half-life in water and log $K_{ow}$ for a given log $K_{aw}$ value. For all of these simulations the half-life in air (48 hours) and half-life in soil ($1 \times 10^6$ hours) were kept constant. The TE boundary is not shown on these plots as, in all cases, the water TE was well below the TE boundary and including the boundary on the plots results in a loss of detail.
This series of simulations clearly show that, in contrast to the overall TE, the water TE clearly increases as the half-life in water increases. The water TE is also relatively independent of the log $K_{aw}$ assumed for log $K_{ow} <5$. The estimated water TE in these simulations is generally low (1%) and reaches a maximum for log $K_{aw}$ of around -3. The longest half-life in water assumed in these simulations is 15,360 hours (640 days) and the results suggest that the estimated TE would be higher for higher assumed half-lives.

d) Water TE – effect of log $K_{aw}$ and log $K_{ow}$ water for a given half-life in water

The fourth series of plots show how the water TE varies with the assumed log $K_{aw}$ and log $K_{ow}$ for a given half-life in water. For all of these simulations the half-life in air (48 hours) and half-life in soil (1×10^6 hours) were kept constant. Again, the TE boundary is not shown on these
plots as, in all cases, the water TE was well below the TE boundary and including the boundary on the plots results in a loss of detail.

This series of plots shows the same general trends as found in simulation c) above, and clearly show the maximum in the estimated water TE at a log $K_{aw}$ of around -3 for substances with log $K_{ow}$ values <5, and that the water TE increases with increasing half-life in water.

**Figure 26**  Effect of log $K_{aw}$ and log $K_{ow}$ on the water TE for a given half-life in water

e) Overall CTD– effect of half-life in water and log $K_{ow}$ for a given log $K_{aw}$

The fifth series of plots show how the overall CTD varies with the assumed half-life in water and the log $K_{ow}$ for a given log $K_{aw}$ value. For all of these simulations the half-life in air (48 hours) and half-life in soil (1×10⁶ hours) were kept constant.
This series of plots show that the overall CTD is effectively independent of the log $K_{ow}$ for substances with log $K_{ow}$ of 5 or below. For substances with log $K_{ow} < 5$, the overall CTD is independent of the assumed half-life in water for log $K_{aw}$ values between 0 and -3 but below this range the overall CTD shows an increasing trend with the assumed half-life in water. This latter finding can be interpreted in terms of the overall CTD for substances with log $K_{aw}$ values down to around -3 being governed mainly by their transport via the atmosphere but at lower log $K_{aw}$ the CTD is increasingly governed by transport via the water phase (this is confirmed by interrogation of the raw data from the model output). Thus a combination of decreasing log $K_{aw}$ and increasing half-life in water results in a change from transport via air to transport via water.
f) Overall CTD– effect of log $K_{aw}$ and log $K_{ow}$ for a given half-life in water

The sixth series of plots show how the overall CTD varies with the assumed log $K_{aw}$ and log $K_{ow}$ for a given half-life in water. For all of these simulations the half-life in air (48 hours) and soil ($1 \times 10^6$ hours) was kept constant.

This series of plots show that, for a given log $K_{aw}$, the overall CTD is effectively independent of the log $K_{ow}$ up to a log $K_{ow}$ of around 5, and within this range the overall CTD reaches a maximum at a log $K_{ow}$ of around -3 when the half-life in water is up to 7,680 hours. At a longer half-life in water, the overall CTD for substances with log $K_{ow}$ values <5 increases with decreasing log $K_{aw}$ for log $K_{aw}$ values <-3. These findings are again consistent with the overall CTD for substances with log $K_{aw}$ values down to around -3 being governed mainly by their transport via the atmosphere but at lower log $K_{aw}$ the CTD is increasingly governed by transport via the water phase. At log $K_{ow}$ values >5, the overall CTD becomes more dependent upon the log $K_{ow}$ at a given log $K_{aw}$, but is relatively independent of the assumed half-life in water.

**Figure 28** Effect of log $K_{aw}$ and log $K_{ow}$ on the overall CTD for a given half-life in water
g) Water CTD – effect of half-life in water and log K_{ow} for a given log K_{aw}

The seventh series of plots show how the water CTD varies with the assumed half-life in water and the log K_{ow} for a given log K_{aw}. For all of these simulations the half-life in air (48 hours) and half-life in soil (1×10^6 hours) were kept constant.

**Figure 29** Effect of half-life in water and log K_{ow} on the water CTD for a given log K_{aw}

This series of plots shows that for log K_{aw} value the water CTD is relatively independent of the assumed half-life in water for log K_{aw} values in the range 0 to -3. This suggests that volatilisation from water with subsequent transport via air is the predominant transport process for these substances, and that the water CTD is governed mainly by the persistence in air rather than water. For log K_{aw} values below this range, there is an increasingly marked dependence of the water CTD on the assumed half-life in water. For log K_{aw} <−3, the water CTD increases with increasing half-life in water for log K_{ow} values below around 6, but for higher log K_{ow} values the water CTD is effectively independent of the log K_{ow}. This suggests that for
substances with log $K_{aw} < -3$ and log $K_{ow} < 6$, the CTD is mainly governed by transport in water, whereas for substances with a log $K_{aw} < -3$ and log $K_{ow}$ of 6 or more, the CTD is mainly governed by volatilisation and transport via the air.

h) Water CTD – effect of log $K_{aw}$ and log $K_{ow}$ for a given half-life in water

The eighth series of plots show how the water CTD varies with the assumed log $K_{aw}$ and log $K_{ow}$ value for a given half-life in water. For all of these simulations the half-life in air (48 hours) and soil (1×10^6) was kept constant.

This series of plots again demonstrates the dependence of the water CTD on the log $K_{aw}$. For a given half-life in water, the water CTD is independent of both the log $K_{aw}$ and log $K_{ow}$ for half-lives in water of 1,920 hours and below. At longer half-lives in water, the water CTD increases with decreasing log $K_{aw}$, particularly for log $K_{aw}$ values of -3 or below, with this increase being more marked as the persistence in water increases.

**Figure 30** Effect of log $K_{aw}$ and log $K_{ow}$ on the water CTD for a given half-life in water

i) Water Pov – effect of half-life in water and log $K_{ow}$ for a given log $K_{aw}$

The ninth series of plots show how the overall persistence in water, Pov, varies with the assumed half-life and log $K_{ow}$ value for a given log $K_{aw}$. For all of these simulations the half-life in air (48 hours) and soil (1×10^6 hours) was kept constant.
This series of plots shows that the water Pov increases with increasing half-life in water for a given log $K_{aw}$. The water Pov is relatively independent of the log $K_{ow}$ for log $K_{ow}$ values up to around 6, after which the water Pov increases with increasing log $K_{ow}$ at log $K_{aw}$ values of -1 or above. At lower log $K_{ow}$ values, a more complex dependence upon the log $K_{ow}$ is evident. The water Pov is also relatively independent of the log $K_{aw}$ value for log $K_{aw}$ values down to around -3, and then increases with decreasing log $K_{aw}$ values at or below this value.

**Figure 31** Effect of half-life in water and log $K_{ow}$ on the water Pov for a given log $K_{aw}$

j) Water Pov—effect of log $K_{aw}$ and log $K_{ow}$ for a given half-life in water

The tenth series of plots show how the water Pov varies with the assumed log $K_{aw}$ and log $K_{ow}$ value for a given half-life in water. For all of these simulations the half-life in air (48 hours) and soil ($1 \times 10^6$ hours) was kept constant.
This series of plots again demonstrates that, for a given half-life in water, the water Pov is relatively independent of the log K_{aw} value for log K_{aw} values down to around -3, and then increases with decreasing log K_{aw} values at or below this value. This increase in the water Pov becomes more marked as the assumed half-life in water increases above 3,840 hours.

**Figure 32** Effect of log K_{aw} and log K_{ow} on the water Pov for a given half-life in water

**Summary of Part 2**

The more detailed modelling carried out in Part 2 of this Annex reveals the following.

- Predictions of TE, CTD and Pov are effectively independent of the log K_{ow} up to a log K_{ow} of around 6.
- The overall TE is effectively independent of the assumed half-life in water over the range tests. The overall TE for substances with log K_{ow} of 5 or below shows a maximum at a log K_{aw} of around -6. The overall TE reflects transport mainly via the air and is governed more by the persistence in air than the persistence in water in these simulations.
- For substances with log K_{ow} values of 5 or below, the overall CTD is effectively independent of the log K_{aw} values for log K_{aw} values between 0 and around -3, but below this log K_{aw} range the overall CTD shows an increasing trend with the assumed half-life in water. This is consistent with overall CTD for substances with log K_{aw} down to around -3 being governed mainly by transport via the atmosphere but at lower log K_{aw} values the overall CTD is increasingly governed by transport via the water phase.
• The water TE for substances with log K_{ow} of 5 or below shows a maximum at a log K_{aw} of around -3 and, in contrast to the overall TE, the water TE increases as the half-life in water increases. The maximum at a log K_{aw} of -3 is likely to reflect two competing processes: a) the potential for volatilisation from water increasing as the log K_{aw} increases, and b) the potential for re-deposition increases as the log K_{aw} decreases. The dependence on the half-life in water is interpreted in terms of a higher build up in the water phase for more persistent substances, resulting in a higher “pool” of substance for volatilisation.

• For substances with log K_{ow} values below around 6, the water CTD is relatively independent of the assumed half-life in water for substances with log K_{aw} values in the range 0 to -3. Below this log K_{aw} range the water CTD for substances with log K_{ow} values <6 shows an increasing trend with increasing half-life in water, particularly when the half-life is longer than 3,840 hours (160 days). Again, this is consistent transport mainly via the air for substances with log K_{aw} of -3 and above, and for substances with log K_{aw} transport via water becomes increasingly important.

• For substances with log K_{ow} values <6, the water Pov is relatively independent of the log K_{aw} value for log K_{aw} values down to around -3, and then increases with decreasing log K_{aw} value at or below this value. This increase in the water Pov becomes more marked as the assumed half-life in water increases above 3,840 hours (160 days). Again, this is consistent transport mainly via the air for substances with log K_{aw} of -3 and above, and for substances with log K_{aw} transport via water becomes increasingly important.

Overall, it can be concluded that for substances with log K_{aw} values above around -3, the mobility in terms of long-range transport, is governed mainly by transport via the air and so the mobility is dependent mainly on the persistence in the atmosphere rather than persistence in water. For substances with log K_{aw} values of -3 or below, the persistence in water becomes increasingly important to the mobility, and this becomes increasingly marked as the half-life in water exceeds around 180 days.
Part 3. Investigation of the effects of log $K_{aw}$ and degradation half-life in soil

Runs of the OECD POV and LRTP Screening Tool were undertaken to investigate the effects of log $K_{aw}$ and degradation half-life in soil of the mobility of chemicals within this modelling framework. The Screening Tool was run by varying the input data within the following ranges.

<table>
<thead>
<tr>
<th>Property</th>
<th>Range/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>200 g/mole (same value used in all model runs)</td>
</tr>
<tr>
<td>Log $K_{aw}$</td>
<td>-7 to 0</td>
</tr>
<tr>
<td>Log $K_{ow}$</td>
<td>-3 to 10</td>
</tr>
<tr>
<td>Half-life in air</td>
<td>48 hours (same value used in all model runs)</td>
</tr>
<tr>
<td>Half-life in water</td>
<td>960 hours (40 days; same value used in all model runs)</td>
</tr>
<tr>
<td>Half-life in soil</td>
<td>960 to 15,360 hours (40-640 days)</td>
</tr>
</tbody>
</table>

Plots showing how the predicted transport efficiency (TE) and the overall persistence (Pov) resulting from release to soil, and how these predictions vary with the assumed chemical property data are shown below. Note: for release to soil the OECD Pov and LRTP Screening Tool does not calculate a characteristic travel distance (CTD).

In each case the legend in the plot has the following format: Log $K_{aw}$, x hrs, where log $K_{aw}$ relates to the log $K_{aw}$ value assumed, x is the assumed half-life in soil in hours. In all runs the half-life in air was set to 48 hours and the half-life in soil was set to 960 hours (40 days).

The Pov plots also show the relevant Pov “boundary” used in the OECD POV and LRTP Screening Tool for identifying substances with POP-like behaviour. If the Pov calculated for a substance is above this boundary, then the substance shows POP-like behaviour.

Please note, in some model runs, very similar results were obtained from some combinations of properties assumed and so only one line is shown on the plots. Where this occurs, the other combinations referred to in the legend lead to essentially the same results as those shown.

a) Soil TE – effect of half-life in soil and log $K_{ow}$ for a given log $K_{aw}$

The first series of plots show how the soil TE varies with the assumed half-life in water and log $K_{ow}$ for a given log $K_{aw}$ value. For all of these simulations the half-life in air (48 hours) and half-life in water (960 hours) were kept constant. The TE boundary is not shown on these plots as, in all cases, the soil TE was well below the TE boundary and including the boundary on the plots results in a loss of detail.

These plots show that the soil TE is effectively independent of the log $K_{ow}$ up to a log $K_{ow}$ of around 3, above which it decreased with increasing log $K_{ow}$. The soil TE shows only a small dependency on the assumed half-life in soil for log $K_{aw}$ down to around -2; at lower log $K_{aw}$ the soil TE shows a more marked increase with increasing half-life in soil.
Figure 33  Effect of half-life in soil and log K_{aw} on the soil TE for a given log K_{aw}

b) Soil TE – effect of log K_{aw} and log K_{ow} water for a given half-life in soil

The second series of plots show how the soil TE varies with the assumed log K_{aw} and log K_{ow} for a given half-life in soil. For all of these simulations the half-life in air (48 hours) and half-life in soil (960 hours) were kept constant. Again, the TE boundary is not shown on these plots as, in all cases, the soil TE was well below the TE boundary and including the boundary on the plots results in a loss of detail.

These plots show that the estimated soil TE reaches a maximum at a log K_{aw} of -3 and that this maximum value increases as the persistence in soil increases. Similar to the case with water (discussed in Part 2 of this Annex) this is suggestive of soil effectively acting as a “reservoir” for volatilisation to the atmosphere, with the potential for volatilisation increasing as the log
$K_{aw}$ increases but the potential for subsequent deposition in remote regions increasing as the log $K_{aw}$ decreases.

**Figure 34** Effect of log $K_{aw}$ and log $K_{ow}$ on the soil TE for a given half-life in soil

![Graphs showing the effect of log $K_{aw}$ and log $K_{ow}$ on soil TE for different half-lives.](image)

c) Soil Pov – effect of half-life in soil and log $K_{ow}$ for a given log $K_{aw}$

The third series of plots show how the overall persistence in soil, Pov, varies with the assumed half-life in soil and log $K_{ow}$ value for a given log $K_{aw}$. For all of these simulations the half-life in air (48 hours) and water (960 hours) was kept constant.

The plots show that for substances up to a log $K_{ow}$ of around 3 the soil Pov is effectively independent of the half-life in soil for substances with log $K_{aw}$ values above -2. At higher log $K_{ow}$ values the soil Pov becomes increasing dependent on the half-life in soil, and the log $K_{ow}$ value at which this dependence on the half-life starts declines as the log $K_{aw}$ declines, such that at a log $K_{aw}$ of -7, the soil Pov for substances with a log $K_{ow}$ value above 1 shows a dependence on the half-life in soil. This is again consistent with volatilisation from soil for lower log $K_{ow}$ values and higher log $K_{aw}$ values, with this becoming less prevalent as the log $K_{ow}$ value increases and/or the log $K_{aw}$ value decreases.
d) Soil Pov– effect of log $K_{aw}$ and log $K_{ow}$ for a given half-life in soil

The fourth series of plots show how the water Pov varies with the assumed log $K_{aw}$ and log $K_{ow}$ value for a given half-life in soil. For all of these simulations the half-life in air (48 hours) and water (960 hours) was kept constant.

This series of plots shows more clearly the effect of the log $K_{aw}$. In all cases the soil Pov increases as the log $K_{aw}$ decreases, and the soil Pov for substances with log $K_{ow}$ values of 2 and above increases as the half-life in soil increases.
Summary of Part 3

The soil modelling carried out in Part 3 of this Annex reveals the following.

- Predictions of soil TE and soil Pov are effectively independent of the log \( K_{ow} \) up to a log \( K_{ow} \) of around 2.
- The soil TE shows a maximum at a log \( K_{aw} \) of around -3 and the soil TE increases as the half-life in soil increases. Similar to the case with water in Part 2, the maximum at a log \( K_{aw} \) of -3 is likely to reflect two competing processes: a) the potential for volatilisation from soil increasing as the log \( K_{aw} \) increases, and b) the potential for re-deposition increases as the log \( K_{aw} \) decreases. The dependence on the half-life in soil is interpreted in terms of a higher build up in the soil phase for more persistent substances, resulting in a higher “pool” of substance for volatilisation.
- For substances with a log \( K_{ow} \) of 3 or below and a with a log \( K_{aw} \) value of -2 and above, the soil Pov is effectively independent of the half-life in soil. At higher log \( K_{ow} \) values or lower log \( K_{aw} \) values the soil Pov becomes increasingly dependent on the half-life in soil. This is again consistent with volatilisation from soil from substances with lower log \( K_{ow} \) values and higher log \( K_{aw} \) values, with this becoming less prevalent as the log \( K_{ow} \) value increases and/or the log \( K_{aw} \) value decreases.