Persistent Organic Pollutants (POPs)
Response to UNEP/INC/CEG-I
Annex 1

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Contents

SUMMARY

An ECETOC task force started to work on the definition of scientific criteria for POP identification in May 1998. UNEP started to work on this issue in July 1998 and a Criteria Expert Group (CEG) established by UNEP met in Bangkok in October 1998 and in Vienna in June 1999 to determine scientific criteria for POPs. The results of the ECETOC TF can be considered as an answer to the first document produced by CEG1 and have been submitted at the CEG2 meeting to help the general discussion on criteria.

A compound has to be peristent, bioaccumulable, long-range transported and show reasons for concern to be nominated as a candidate POP. If nominated, a compound will need to go through a risk assessment to conclude if it has to be included or not in the protocol on POP.

For the nomination step the ECETOC TF has concluded :

That a $^1/_2$life of 6 month is an acceptable value for the persistence criteria in soil, sediment and water based on information on existing POPs and the relation between environmental compartments. For compounds which are not readily biodegradable existing 28-day standard tests are not sufficient to measure persistence in relation to the specific needs of the protocol on POP. Adequate methodology and tests will have to be defined.

Regarding bioaccumulation, the value of $\log K_{ow}$ should range between 5 and 8 for the compound to be considered. These limits are dictated by the data available on correlation between $\log K_{ow}$ and BCF values which show that outside this range the BCF will be less than 5000.

The long-range transport and deposition can be studied on the basis of physicochemical properties e.g. the sub-cooled liquid vapour pressure of the compound. It is shown for example that lipophilic compounds with sub-cooled liquid vapour pressures higher than 1 pa will stay mainly in the atmosphere and will not be deposited.

The methodology to define the reasons for concern is by comparing observed or expected concentrations in the environment with toxicological and or ecotoxicological data.

As a general consideration, the ECETOC TF concluded that priority should be given to quantitative criteria.

For the evaluation stage :

A clear need is emerging for a generally accepted multi-media model capable of predicting persistence and long-range transport in the environment. The model will need to take into account the variability of environmental conditions and the different exchanges between the environmental compartments which cannot be considered by single numbers for each compartment as in the case of the persistence criteria.

1. INTRODUCTION

Persistent organic pollutants (POPs) are substances which resist abiotic and biotic degradation, may bioaccumulate, can be transported over long distances and can potentially cause adverse effects to either humans or ecosystems. The long-range transport and deposition of such substances and the resulting potential for their widespread distribution has made the POP issue one of global concern.

The issue was first addressed by the UNECE (United Nations Economic Commission for Europe) convention on long-range transboundary air pollution and later on by UNEP (United Nations Environmental Programme). Initially twelve substances, nine of which were pesticides that became widely used in the late 1940s, were targeted in the POPs treaty negotiations. In July 1998 UNEP started the process to develop a protocol for POPs. A criteria expert group (CEG) was commissioned to define the scientific criteria needed to identify POPs.

An ECETOC TF was established in 1998 to address the scientific criteria for priority setting and assessment of persistent organic pollutants, the conclusions of which will be issued as a detailed technical report during 2000 as a contribution to the international debate.

Members of this TF were also invited to the CEG meetings and were thus able to propose criteria for the nomination step for POPs and a framework for the risk profile stage that will follow any identification of a candidate POP.

The objective of this interim document is to detail the ECETOC response to Annex 1 'Information requirements and criteria for the nomination and screening stage and for the evaluation stage' produced by CEG-1 (UNEP/INC/CEG-1). Each step of the document produced at CEG-1 has been reviewed. To facilitate the understanding of this paper, the sentences from the CEG-1 document are reproduced in italics. When the scientific material needed to support the comments requires some development, this is done in corresponding appendices.

The ECETOC TF concluded that priority should be given to using quantitative criteria at the nomination stage and that statements used in the CEG-1 document not supported by quantitative criteria should be made more accurate.

2. CRITERIA FOR POP

2.1 Nomination stage

2.1.1 Persistence

(b) Persistence: Evidence that the substance's half-life[3][4], in water is greater than [2 months] [6 months], or that its half-life[3][4] in soils is greater than six months, or that its half-life[3][4] in sediments is greater than six months;

[3] Conditions and methods of measurements need to be defined.
[4] It is preferable to use substance half-life based on degradation, not disappearance into another compartment.

In the persistence section of the CEG-1 document, it is proposed to consider 2 or 6 months for the persistence in water and 6 months for the persistence in soil and sediments. It is also indicated in the footnote 3 that "conditions and methods of measurements need to be defined".

The persistence criteria for water should be a half-life of 6 months, the same as for soil and sediment, for the following reasons:

- Data given in the ICCA position paper (ICCA, April 1998) show that the persistence of existing POPs in soil, water and sediment would be of the order of 1 year or more. Therefore, the value of 6 months could be considered as a conservative value;
- The USA EPA (Boethling *et al*, 1995) analysed the biodegradation database for a number of chemicals and they concluded that aerobic degradation rates were similar for water and soils. Sediment and water are directly linked (SETAC, 1999). A chemical will partition rapidly between the two phases, and furthermore a multi-media model (such as will be needed for the later stages of the evaluation) will assume that the concentrations in the water and sediment phases in the aquatic compartment are at or near equilibrium. Degradation in one phase will result in a decline in concentration in the other, as equilibrium is re-established;
- Existing sediment test methods incorporate a water phase and do not distinguish between degradation of sediment bound and dissolved material (SETAC, 1999; OECD, 1998);
- Regarding the measure of persistence in soil, water and sediments, there is support for the statement in the footnote 3 indicating the need to work on test methods.

Experimental data for most nomination chemicals will relate to conventional studies (e.g. 28-day studies) which were not designed to measure the biodegradation of chemicals with half-lives of up to six months. Maximum use should be made of the available data and therefore some extrapolation will be necessary. For example compounds already identified as biodegrading easily in standard tests will have half-life values shorter than the proposed criteria. As stated by UNEP (POPS/INC 1/6), persistent chemicals would constitute only a small sub-set of those which are not easily biodegradable. Failure to meet the criteria for biodegradability in a standard test should not mean that the substance is considered to have a half-life higher than 6 months. In many cases such substances may show significant biodegradation within the relatively short test period.

These data should be examined on a case by case basis but will often be sufficient to indicate a half-life of less than 6 months. Failure to show any significant biodegradation in these tests, does not necessarily indicate a half-life of more than 6 months. In such cases, or if no test has been carried out, then the use of an appropriate structure-activity relationship (SAR) (particularly based on field data) may be useful at the nomination stage. However if the existing experimental data are inconclusive it may be necessary at the evaluation stage to generate half-life data over a longer observation period in a test designed to address the POP's persistence criteria.

Degradation by both abiotic and biotic routes should also be considered in combination when assessing against the persistence criteria. In this respect not only standard tests but all reliable study data should be used.

There is scientific support to recommend that at the evaluation stage, a global persistence be derived using multi-media modelling. Transport to other compartments followed by degradation in these compartments, which may be the only removal process in some media, is ignored if half-life considerations are restricted to individual compartments. For adequate consideration of this removal mechanism, multi-media modelling is certainly a possible approach. The model approach could also reflect variations in temperature, sunlight, microbial community variations and differences in the release pattern which strongly affect the fate of substances in the environment and consequently their global persistence. The evaluation of global persistence should be carried out with a multi-media model validated with a broad range of chemicals.

2.1.2 Bioaccumulation

(c) Bioaccumulation:[5] Evidence that the BCF or BAF in aquatic species for the substance is greater than 5,000 or in absence of BCF/BAF data, the logK_{ow} is greater than [4][5][6]

[5] The contact group considered that for the evaluation stage logK_{ow} is not sufficient to make a thorough evaluation of bioaccumulation potential.

[6] When the bioaccumulation potential is based on the logK_{ow}, effects of molecular dimensions, molecular weight, metabolic potential, and solubility may need to be considered.

The value for BCF of >5000 (log BCF >3.7) is appropriate to identify substances with substantial bioaccumulation potential. The appropriate and corresponding value for logK_{ow} is 5. ECETOC (1995) cites the two most commonly used relationships between log BCF and logK_{ow}

Log BCF = logK_{ow} – 1.32 (Mackay, 1982)

Log BCF = 0.79 logK_{ow} – 0.4 (Veith and Kosian, 1983).

There is also recent work from Bintein *et al* (1993) describing a non-linear relationship.

Log BCF = 0.91 logK_{ow} – 1.975 log (6.8E-7 K_{ow} + 1) – 0.786

These indicate logK_{ow} values of 5.0 and 5.2 and 5.0, respectively, as predictive of a BCF of 5000.

With respect to footnote 6 there is scientific support to propose an upper value for the logK_{ow}.

There is clear evidence from experimental work that superlipophilic compounds ($logK_{ow}$ >7.2, Bintein *et al*, 1993) and substances of high molecular weight (> 700, Technical Guidance Document, 1996) do not show significant bioaccumulation (see appendix B). For instance, the bioaccumulation potential decreases above a $logK_{ow}$ of 7.5 and is hardly detectable above a $logK_{ow}$ of 8.

Therefore it is proposed that the criteria should be 'the $logK_{ow}$ is between 5 and 8'.

2.1.3 Long-range Transport

Environmental fate properties[7] and/or model results that demonstrate that the substance has a potential for long-range transport [and potential exposure] through air or water or migratory species [and deposition in locations distant from the sources of release of the substance]. For substances that migrate significantly through the air, the air half-life should be greater than 2 days;

[7] Environmental fate properties and data relevant for assessing long-range transport which may also be used in models include physical and chemical characteristics of the substance such as vapour pressure, Henry's law constant, other partition coefficients; half lives in various media; studies relevant to persistence etc. The model approach needs to be further explored.

- In the case of substances that migrate through the atmosphere, deposition is a key property which enhances the potential for exposure far away from the source. The TF suggest that the parenthesis be removed from around the phrase 'and deposition in locations distant from the sources of release of the substance'.
- In the case of lipophilic substances transported via air there is evidence that for sub-cooled liquid vapour pressure > 1 Pa, deposition would not occur and for sub-cooled liquid vapour pressure smaller than 10^{-4} Pa, deposition would take place locally (see appendix C). For such substances long-range transport and deposition will occur for sub-cooled liquid vapour pressure ranging between 10^{-4} and 1 Pa. These indications could usefully be added in the case of substances that migrate significantly through the air.
- Predicting long-range transport and deposition of chemicals, because of the high variability of environmental conditions and interaction between media, should be done using appropriate multi-media modelling. Therefore it is recommended, as in the case of the persistence criteria, that a multi-media model be developed to assess transport and deposition potentials at the evaluation stage.

2.1.4 Reasons for Concern

e) Reasons for concern: Evidence that [chronic] toxicity or ecotoxicity data, compared where possible with available detected or predicted levels of a substance, indicate a potential for damage to human health or the environment caused by the substance resulting or anticipated from long-range transport.

A "potential for damage" can only be indicated by comparison of the toxicity data with the detected or predicted concentrations in the environment, because hazard data alone are not sufficient to cause "concern" unless related to exposure. A preliminary quantitative, rather than qualitative, comparison of toxicity and exposure should be provided for the nomination stage, so that the level (degree) of concern is transparent. In this condition the words "*where possible*" should be deleted and consequently the proposed wording is as follows:

"e) **Reasons for concern:** Evidence that [chronic] toxicity or ecotoxicity data, compared quantitatively with available detected or predicted levels of a substance, indicate...."

3. RISK PROFILE

3.1 Background

The CEG-1 report, (UNEP/POPS/INC/CEG/1/3) and specifically Annex II, recommended that there be a full risk evaluation/review for a substance that has passed through the initial prioritisation and review step. This full risk evaluation/review would be summarised in a "Risk Profile", the content/scope of which should be defined. ECETOC presents this document as a scientific contribution to the process of defining the minimum information required to elaborate a "Risk Profile", which could be used as a basis for further decisions and risk reduction measures.

3.2 Contents of the "Risk Profile" document

The first part of the "Risk Profile" should contain a summary of the key relevant data on the substance:

- physical, chemical, and degradation properties;
- potential effects on humans and biota and the concentrations of concern;
- environmental fate;
- measured environmental concentrations and/or biota including humans, particularly in areas far away from the emission sources.

To ensure transparency and openness, the quality of the available data should be reviewed on the basis of internationally accepted criteria for assessing the validity of effect and others measured data, such as those developed by the OECD/IPCS. The objective of this review is to select those data that are of the best quality and most relevant for the full risk evaluation/review. Those data, which have a significant influence on the outcome of the "Risk Profile" should particularly be submitted to an in-depth evaluation.

Two different types of data are needed for the characterisation of both hazard and exposure.

In **hazard evaluation**, there is a need, not only for a review of the overall quality of the laboratory, clinical or field data, but also for a clear description of the kind of adverse health and environmental effects, which have been observed. Particular emphasis will be put on effects related to the survival, growth and reproduction of humans and populations of organisms in the environment. Of course, the range in concentrations associated with each observed adverse effects should be specified. A separate evaluation of the hazard data for human health and the environment is needed due to the different populations and organisms affected.

In **exposure evaluation**, a preference should be given to monitoring data, provided that their quality and representativeness have been checked (ECETOC, 1999). A particular emphasis should be given to concentrations observed in biota or in human tissues far away from the emission sources or in remote areas like in Arctic and Antarctic regions.

In modelling approaches, the quality of the physical, chemical and degradation data used as parameters in the models should be checked and the model itself should be validated. Similarly, production levels, type of uses and importance of releases should be critically analysed before being used in modelling approaches. Finally, the probable fate and exposure pathways should be realistic and indicative of a possible long-range transport process. The measured and / or calculated exposure concentrations should be compared to the concentration range where effects could occur, as described in the hazard assessment section.

In such a comparison only the bioavailable fraction of the substance should be considered in the exposure level. It is also important in this evaluation to recognise that human and wildlife exposures are likely to be substantially higher through the food chain than through direct contact; therefore, persistence and bioaccumulation potential are often critical factors influencing likelihood and magnitude of exposure.

In the second part of the "Risk Profile" the conclusions of the expert group should be summarised.

These will focus on determining the likelihood of significant adverse effects on human health or the environment from past, current and / or continued future use of the substance due to its long-range transboundary transport.

This evaluation will use:
- existing risk assessments for the substance;
- information on hazard and exposure that was summarised in the first part of the report;
- expert judgement.

In recognition of the wide variability in conditions and exposures globally, the results of the expert evaluation would be summarised primarily as probability ranges. For example, for a given effect endpoint, the summary would indicate the likelihood of occurrence and the severity and reversibility of an effect under reasonably foreseeable conditions of exposure. The strength of this conclusion should be based on the quality of the data used. The profile would then determine the likelihood that the distribution of exposures overlaps with the distribution of concentrations that have been found to result in specific toxic effects. Throughout the evaluation, it is important that the magnitude of exposure and effects should consider both the original substance and any breakdown products with POP-like characteristics.

3.3 Control measures

The results of the risk profile and some considerations of the risk and benefit of the substance in question combined with an analysis of socio-economic aspects should be the basis for determining the level of controls that are appropriate and reasonably achievable. With this information the exposure evaluation could be re-assessed to determine whether the proposed controls will reduce the likelihood of significant adverse human health and / or environmental effects (i.e. risk) from the substance to an acceptable or adequate level.

APPENDIX A: PERSISTENCE

A.1 Persistence in water, soil and sediments

Persistence has been identified as one of the criteria that should be used to nominate compounds as a candidate POP. It is therefore necessary to study how persistence can be best defined, how it can be best measured and finally indicate some directions of scientific work that might be needed for the future.

Persistence should indicate the rate at which a substance may disappear by degradation from the environment. It is generally expressed as the half-life, which is the time required for the concentration to reach half of its initial value.

The persistence can be defined for a given medium i.e. water or soil or sediment. Global persistence can also be defined which takes into account all the different interactions between the environmental compartments (i.e. water, soil, sediments, air).

A.1.1 How to Measure Persistence in a Given Medium (Water, Soil and Sediments)

First, it is important to note that maximum use of existing data should be made at the nomination stage. Substances that easily biodegrade in the existing 28-day tests will not persist in the environment. Substances that cannot be classified as easily biodegradable but show some biodegradation are likely to have a half-life under environmental conditions shorter than the POPs persistence criteria. Some work on how data might be extrapolated to environmental condition is however necessary. (SETAC, 1999).

For compounds for which existing 28-day tests or structure-activity relationship would not give enough information, there is certainly a need to develop testing conditions over longer periods closer to environmental conditions. This is supported by the fact that it is difficult to derive degradation kinetic information from standard tests.

OECD and ISO have developed test methods for both primary and ultimate biodegradability (OECD, Technical Report ISO / TR 15462, 1998 (E)). Many tests and test data are available and a large number of these have been the subject of ring tests. Subsequently the EC adopted the methods for use in conjunction with the notification of new chemical substances and the testing requirements for prioritising existing substances.

As a result of the ring tests, the methods were classified as being suitable for assessing ready biodegradability, inherent biodegradability or the degree of degradation in tests simulating activated sludge processes. However, it has been concluded that the methods for ready biodegradation as written, offer limited opportunity of calculating kinetic constants (Painter, 1996).

Chemicals which degrade well in the aerobic ISO 'ready' tests can be expected to undergo rapid ultimate degradation in the environment. Chemicals which fail the ready tests (the tests using lower cell densities) and degrade only in those laboratory tests with a higher biodegradation potential (e.g. inherent tests), will also be expected to be ultimately biodegradable in the environment. Degradation in the environment is dependent upon the presence of microorganisms with the appropriate catabolic pathways.

This capacity to biodegrade a substance is in turn related to the time and level of exposure of the microorganisms to the substance.

Similarily, chemicals which degrade in the more powerful tests (ISO 9887 and ISO 9888) may not necessarily degrade in the activated sludge simulation test, probably because the sludge has not been adapted to the test compound, while other chemicals do. Different pathways exist for biodegradation in aerobic and anaerobic environments and both these potential routes should be considered in an assessment of persistence.

Battersby (1990) and ECETOC (1991) both concluded that the tests likely to yield the most relevant results will be those closely reproducing conditions in the environment under consideration; tests for ready biodegradability do not match this requirement, and therefore failure to pass a ready test should not be considered as an indication of persistence. Alexander (1994), who has uncovered many complex kinetic relationships in the natural environment, indicates that studies on the kinetics of biodegradation are often empirical, reflecting a rudimentary level of knowledge about microbial populations and activity in the environment.

At the international workshop on biodegradability of chemicals (UBA, 1983), it was observed that the conditions were so different in the tests compared to those in the environment that any constants derived from laboratory results would not apply in the environment. Relevant environmental conditions cited were the presence of multi-substrates, synergism / antagonism, varying concentrations of substrates, different rates of adaptation. This is all indicative that the determination of the potential persistence of a chemical should be based on a realistic environment or at least on tests with high potential for degradation (incl. adaptation, bacterial mix, etc). This supports the necessity for realistic long-term tests mimicking the environment (e.g. OECD, 1998).

In addition to the role of biodegradation it is important to take into account the abiotic degradation process that may occur i.e. hydrolysis, photolysis and oxido-reduction processes. The half-life of a substance for a given medium will be the result of the combination of all significant biotic and abiotic processes.

A.1.2 The Need to Evaluate Global Persistence

The relevant parameter which is important to understand the potential impact of a substance on the environment remains its persistence under real environmental conditions. The persistence measured as described above may be useful at the nomination step but is not adequate to conclude on how a compound will behave in the environment. This complex issue has been reviewed by Webster *et al*, 1998.

A.1.3 Variability of Environmental Conditions

Physico-chemical conditions can be expected to vary widely in the environment. This means strong variations of temperature, hydroxyl radical concentration in the atmosphere, UV flux, bacteria populations etc. One example given in Webster *et al* (1998) is the rate of atmospheric degradation of tetrachlorobiphenyl as a function of latitude. It is seen that because of temperature and hydroxyl radical concentration variations the atmospheric persistence of that compound is expected to vary within two orders of magnitude.

Table 1: Estimation of the Degradation of a Tetrachlorobiphenyl under Different Environmental Conditions (Webster et al, 1998)

	Temperature (C^0)	**[OH]**[a] (10^6 molecules/cm^3)	**Rate constant** (s^{-1})	**Degradation** (half-life)
Mid-latitude, summer (diurnal average)	15	0.6	5.57e-07	14.4 d
Mid-latitude, winter (diurnal average)	-5	0.06	4.44e-08	180.5 d
Tropical, high noon (maximum)	30	6	6.46e-06	1.2 d
Polar, night (minimum)	-20	0.006	3.67e-09	6.0 y

[a] Hydroxyl radical concentrations are based on Altshuller (1989)

This variability may be expected for other degradation processes such as hydrolysis, biodegradation, photolysis etc. It is therefore probably more appropriate for persistence to be represented by a distribution of values rather than a single number.

A.1.4 Exchange between the Different Environmental Media

The persistence defined for each medium does not take into account the effect of exchange between soil, sediment, water and air and also the compartment where the compound could be preferentially located because of its physico-chemical properties. It does not take into account the mode of introduction of the compound in the environment.

A.1.5 The Need for Multi-Media Modelling

To solve the difficulties explained above, one possibility is to develop appropriate multi-media modelling tools to derive global persistence values in the environment, expressed as a distribution of values reflecting the variability of environmental conditions. This approach has been proposed at the SETAC workshop on persistence and long-range transport (SETAC, 1999).

APPENDIX B: BIOACCUMULATION

B.1 Criteria for criteria for bioaccumulation of POPs

Introduction

Bioaccumulation is defined as the net result of uptake, distribution and elimination of a substance in an organism. It includes all routes of exposure which are principally those across respiratory surfaces and by ingestion of food, water and other material. For aquatic (water breathing) organisms, accumulation from water across the gills (or other respiratory surfaces) is termed bioconcentration; this is the major route of exposure for many substances and is more commonly measured in laboratory studies than bioaccumulation from food. For air-breathing animals, the inhalation route is included, but dietary exposure is generally considered to be more important. Biomagnification is defined as accumulation and transfer of substances via the food web, in particular to express an increase in the concentrations within organisms at successive trophic levels.

ECETOC (1995) reviewed in detail the role of bioaccumulation in the aquatic environment. The principal conclusions are summarised as follows:

- Bioaccumulation of a substance into an organism is not an adverse effect or hazard in itself.
- Bioaccumulation may lead to a body burden which may cause toxic effects on the organism due to water and/or dietary exposure, or may be toxic to its predators.
- Biomagnification is less widespread than commonly believed, only having been demonstrated for a very limited number of substances.
- Metabolism (biotransformation) of the substance may increase the elimination rate and therefore decrease the bioconcentration factor. Rates of xenobiotic biotransformation vary between phyla and species and are a function of general metabolic rate.

The potential of a substance to bioaccumulate is related:

- primarily to its lipophilicity. If measured values of the bioconcentration factor (BCF) are not available, the octanol-water partition coefficient (K_{ow}) may be useful as a predictor of bioconcentration for organic, non-polar substances, although for other substances this may be less reliable.
- to its lack of biotransformation through metabolism
- to its molecular volume or size

Relationship between BCF and K_{ow}

Due to the hydrophobic nature of organic contaminants, their dynamics in the foodchain is closely related to the lipid content of the organisms. Especially in Arctic regions, high lipid levels are found in the organisms as an adaptation to the cold climate and the cyclic annual productivity. Long lipid-based and complex foodchains may contribute to high levels of organic contaminants in the Arctic.

The lipophilicity of a neutral organic substance can be estimated by the octanol/water partition coefficient, K_{ow}, which is often used as a surrogate when no experimental value of the BCF is available.

While bioaccumulation and biomagnification increase with K_{ow} in the range of medium to high lipophilicity, the low solubility and hence low mobility of extremely lipophilic substances inhibits the kinetics of their bioaccumulation as well as of their biomagnification. As already stated, the molecular weight and the molecular diameter also play a role and may influence the bioaccumulation by limiting the diffusion through cell membranes.

In the case of bioconcentration in fish, water solubility, which decreases when K_{ow} is increasing, is one of the main factors limiting the uptake rate. In biomagnification via the food-chain, the absorption efficiency from the intestinal tract into the body decreases when increasing octanol-water partition coefficient.

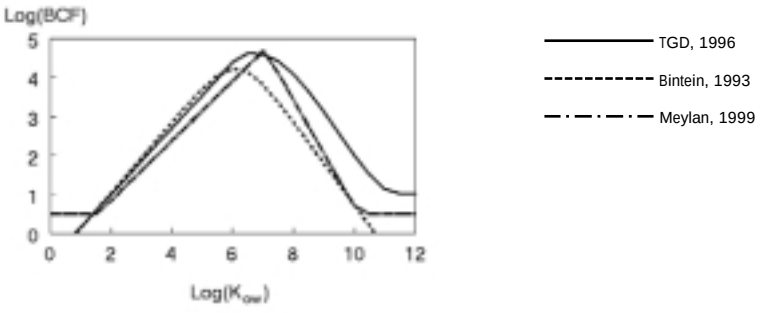
These findings are reflected in a new QSAR programme BCFWIN of the Syracuse Research Corporation in co-operation with the US Environmental Protection Agency (Meylan *et al*, 1999). The following correlations between BCF and K_{ow} are proposed for non-ionic organic substances:

logK_{ow}	**Log BCF**
< 1	0.5
1 to 7	0.77 logK_{ow} - 0.7 + S F_i
> 7	-1.37 logK_{ow} +14.4 + S F_i
> 10.5	0.5

The F_i s are correction factors for specific chemical groups.

The above QSAR shows that the bioconcentration potential (BCF) increases with the logK_{ow} up to a value of 7 and at higher logK_{ow} the BCF does not increase any more but decreases quite steeply. This behaviour is illustrated in Figure 1 hereafter, together with some of the previous work done on correlation between BCF and logK_{ow}.

Figure 1: Bioconcentration factor BCF dependent on octanol/water partition coefficient K_{ow}



These various relationships take into account all the factors which are limiting the bioaccumulation rate of highly lipophilic substances and are generally well accepted. Other views exist however indicating that the decrease in BCF with K_{ow} when $\log K_{ow}$ is higher than 7 is linked to a kinetic effect and not to the potential to bioaccumulate. This potential would remain constant but the time needed to reach the saturation is becoming longer and longer as the K_{ow} value increases. For highly persistent substances, the exposure period could be long enough to reach the equilibrium even for very highly lipophilic substances. To check this hypothesis, measurements of BCF over very long periods of time are needed. On a practical point of view, measurement of concentration in biota in field experiment could give a first answer to this question. For the time being, no strong argument exists to support this view and it is suggested to keep the Syracuse QSAR model to estimate BCF from K_{ow}.

B.2 Influence of the uptake rate

Uptake via the gills in fish

The bioconcentration factor may be considered as the ratio between uptake and elimination rates, in a steady state situation. In this context, is interesting to look at the magnitude of the uptake rate with increasing K_{ow} and increasing molecular weight. Sijm and Linde (1995) have derived a QSAR for the uptake rate in fish via the gills (see equation 1 hereafter)

$$(1)\quad k_1 = \left[M^{0.71} \left(0.424 * W^{0.344} + \frac{147 * W^{0.23}}{K_{ow}} \right) \right]^{-1}$$

in which

M = Molecular weight of the substance
W = Body weight of the fish
K_{ow} = Octanol/water partition coefficient
k_1 = Uptake rate constant ($m^3.kgbw^{-1}.day^{-1}$) where the m^3 refers to the amount of water going through the gills of the fish

This relationship is illustrated in the Figure 2 hereafter for a 500 molecular weight substance and a fish of 200 g.

Figure 2: Variation of the uptake via the gills versus octanol/water partition coefficient

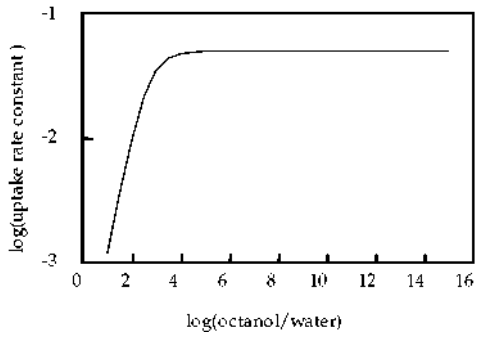
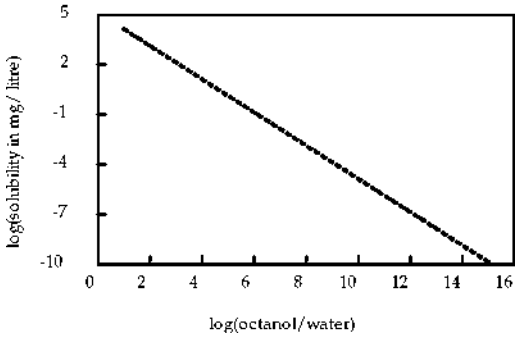


Figure 3: Solubility versus octanol/water partition Molw. 500 Melting Pt 100°C



On the other hand, the solubility of a chemical in water varies with K_{ow} according to the equation 2 hereafter (Mackay, 1982)

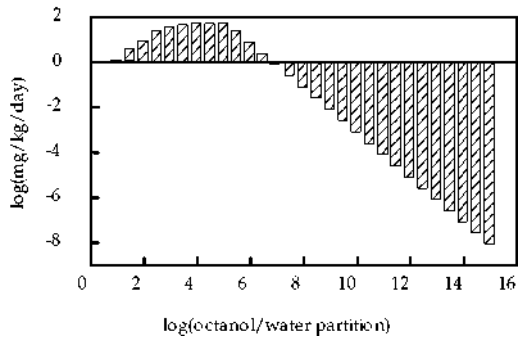
(2) $\ln(C)=7.494-\ln(K_{ow})+6.79(1-T_M/T)$

C = Water solubility in mMol/litre
K_{ow} = Octanol/water partition coefficient
T_M = Melting point in °K
T = Ambient temperature in °K

This relationship is illustrated in Figure 3 for a molecular weight of 500 and a melting point of 100°C.

As k_1 is expressed in m^3 of water going through the gills, by multiplying k_1 by the concentration of the substance in water ,the uptake rate of the substance via the gills, expressed in mg/kg bw/day, can be calculated and plotted as a function of the log (octanol/water partition coefficient). Figure 4 illustrates this relationship, for a molecular weight of 500, a melting point of 100°C, a fish of 200 g, a concentration, which is taken equal to 1000 mg/m^3 = 1 mg/liter or to the water solubility as given by equation 2 if lower than 1mg/l.

Figure 4: Variation of the substance uptake rate via the gills as a function of the octanol/water partition coefficient



From this graph, the K_{ow} value of the substance can be defined at which the uptake rate has fallen to such a low level, that bioconcentration could become negligible. For example, at a log K_{ow} of 10 and a molecular weight of 500, a fish of 200 grams will take up no more than 0.7 µg/kg bw/day. It means that, at constant uptake and zero elimination, a period of 1400 days (about 4 years) is needed for the concentration in a fish of 200 grams (without considering any growth) reaching the same level as in the ambient water phase.

Since elimination rate generally increases with increasing body load, this “equilibrium” will be approached even more slowly.

The fact that superlipophilic compounds do not bioconcentrate very quickly in biota is confirmed by experimental studies. For example, the Chemicals Inspection & Testing Institute Japan (1992) observed, that decabromobiphenyl (estimated [Howard 1995] log(K_{ow})=12.6, mol.weight 943) did not bioconcentrate at all in bioaccumulation tests with carps over a period of 8 weeks. Similarly, Krüger (1988) when studying the occurrence of polybrominated biphenyls and diphenylethers in fish, seals and mother milk, found that octa- nona- and deca-bromobiphenyl were hardly present and, if detectable, present at a much lower level than the lower brominated congeners. This indicates, even in biota at the end of the food chain, a lesser level of uptake of substances with higher K_{ow} values.

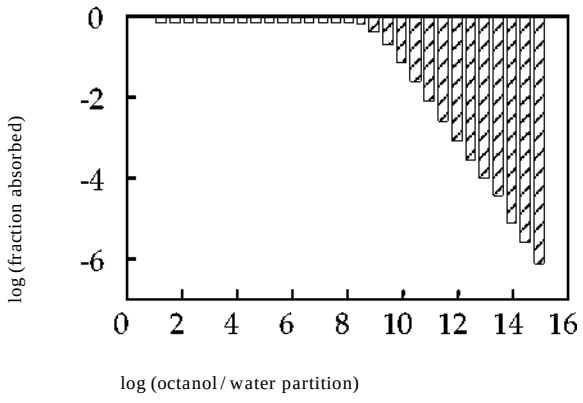
Uptake via the food in fish

The biomagnification factor in fish for hydrophobic compounds with a log(K_{ow}) > 6 and no biotransformation depends on the daily feed volume, the daily faecal volume and the partition coefficient of the hydrophobic compound between feed and faeces. The fat content of the faeces is generally lower than that of the diet, dependent on the digestibility of the food. For this type of compounds, biomagnification factors in fish are mostly in the typical range of 3 to 5 (Gobas *et al*, 1993).

The time required to reach the equilibrium in biomagnification depends on the actual uptake rate in relation to the absorption efficiency from the intestinal tract into the body. Clark *et al* (1990) and Thomann (1989) have discussed the absorption efficiency of chemicals from food as a function of the octanol / water partition coefficient (K_{ow}). From their data, it appears that the absorption efficiency from the intestinal tract into the body decreases with increasing logK_{ow}. One of the equations of Clark *et al* (1990) for the absorption efficiency EA of rainbow trout is presented hereafter (equation 3):

$$(3)\quad E_A = \frac{1}{1.32+1.39E\text{-}9*K_{ow}}$$

Figure 5: Absorption and ingestion of chemicals via feed in rainbow trout



In Figure 5, the fraction absorbed from a chemical in diet is plotted against the octanol / water partition coefficient in the case of rainbow trout. This figure clearly shows that the absorption efficiency strongly decreases with K_{ow}, in particular for substances with a logK_{ow} >8.

If a log K_{ow} value of 12.5 (equal to that of, for example, decabromodiphenyl ether) is considered, the absorption efficiency is estimated to be 2.3E-4. The experimental efficiency derived from a measured absorption of 0.15 mg/kg over 120 days reported by Kierkegaard *et al* (1995) for a daily ingestion of 9 mg/ kg is 1.4E-4, a value which is in a reasonable agreement with the estimated efficiency of 2.3E-4 in rainbow trout as calculated by equation 3. This experiment indicates that the decabromodiphenyl ether can bioaccumulate in fish even if the absorption efficiency from the food is poor. After 120 days exposure, only a very small fraction of the substance ingested via the food (at a concentration of 90 mg/kg) is found in the fish at a level of 0.15 mg/kg. This indicate that a slow rate of absorption does not lead to a biomagnification through the food chain, since this term implies a higher concentration in the target medium than in the source medium.

It has also to be pointed out that the absorption efficiency has been observed to vary between species within an order of magnitude, the rainbow trout being the species with the highest observed absorption efficiency (Clark *et al*, 1990). This can then be considered as a worst case situation for assessing the risk of bioaccumulation.

The octanol-water partition coefficient is not the only parameter controlling the uptake rate of chemical in biota. For instance, steric factors like molecular size and shape could also play a role by limiting the permeation through biological membranes.

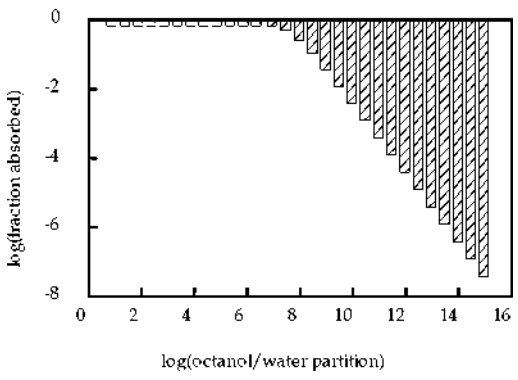
For example hexabromobenzene and decachlorododecane have about the same molecular weight and about the same octanol water partition coefficient but the first one does not bioaccumulate from aqueous solutions into fish, while the second does (Bruggeman, 1983, Sundström and Renberg, 1986). The same applies to octachlorodibenzo-p-dioxin and decachlorobiphenyl respectively. According to Opperhuizen *et al* (1985) this is caused by steric factors. The diameter of molecules like hexabromobenzene and octachlorodibenzo-p-dioxin is assumed to be too big (>0.95 nm) to allow the permeation through biological membranes at a reasonable speed.

B.3 Uptake rate and bioaccumulation in mammals

McLachlan (1994) studied the absorption of hydrophobic contaminants in cows. The fractional absorption Eo of a compound is said to be related to the octanol/water partition coefficient K_{ow} according to the following relation:

$$E_0 = \frac{1}{1.283 + 2.875E\text{-}8 * K_{ow}}$$

Figure 6: Ingestion of chemicals via feed in cattle



In Figure 6 above, the fraction of chemicals adsorbed from diet is plotted against the octanol/water partition coefficient (in log scale) in the case of cattle. This figure clearly illustrates that, in cattle also, absorption from the intestinal tract into the body decreases with increasing $\log K_{ow}$ as previously shown in trout. This is particularly true for $\log K_{ow}$ higher than 8.

To illustrate this effect, the Kow values estimated by the software programme of the Syracuse Research Corporation (Howard, 1995) were used for estimation of the absorption Eo of brominated biphenyl congeners. The K_{ow} values vary from 4.65 to 12.66 when going from mono- to deca-bromobiphenyl, the adsorbed fractions decreasing from 7.79E-01 to 7.61E-06. This could explain why large differences in brominated biphenyl concentrations are observed in lipid tissues of cows.

Due to the fact that absorbed fraction decreases with increasing K_{ow}, the uptake rate and consequently the bioaccumulation is very slow for substances with a K_{ow} greater than 10 Chlorinated paraffins can also be used to illustrate the possible effect of absorption efficiency. Short chain, highly chlorinated paraffins have been shown to be more toxic to the rat than the long chain, less chlorinated ones. Part of this difference may be explained by the fact, that the longer-chain grades are less well absorbed from the rat gut than the shorter-chain grade. The extent of absorption and the metabolism is probably related to the degree of chlorination and most probably to the length of the carbon chain (Serrone *et al*, 1987). It is interesting to note, that with increasing chain length and with increasing chlorination, the octanol/water partitioning is also increasing. The increase of a CH_2-moiety results in a greater increase in K_{ow} than the increase of one chlorine-substitute. In case of short chain chlorinated paraffins the extent of chlorination does not only control the K_{ow} but also the extent of metabolism, the lower the degree of chlorination, the lower the K_{ow} value, the higher the biotransformation rate and the lower the bioaccumulation.

B.4 Conclusions

The bioconcentration and the bioaccumulatiobn of chemicals in living organism is strongly dependent on their lipophilicity as expressed by the octanol/water partition coefficient, K_{ow}. The K_{ow} value is also a key parameter to describe the water solubility of the chemical and its ability to be absorbed from the intestinal tract into the body of various animals.

The lipophilicity of a chemical depends on its molecular weight and on its degree of halogenation. But if the size of the molecule increases, the permeation rate through the cell membrane could be drastically reduced, leading to a significant decrease in the bioaccumulation potential.

Due to the difficulties in establishing a simple relationship between K_{ow} and BCF it is important to give a preference to experimentally determined bioaccumulation potential.

Elimination is a combination of depuration and metabolism – both of these processes need to be taken into consideration when predicting a bioaccumulation potential, and will be fully addressed in the Technical Report prepared by the Task Force.

Appendix C: Long-range Transport

C.1 Long-range transport and deposition

To be considered as a POP, in addition to being toxic, bioaccumulative and persistent, a compound must have such physico-chemical properties that it can be transported over long-range and further deposited. Long-range transport is thought to happen mainly through the atmosphere although other ways are considered i.e. water and migratory species.

Both physico-chemical data and modelling can be used at the nomination stage to determine if a compound potentially can be transported over a long-range.

C.2 Using physico-chemical data

C.2.1 Atmospheric Transport

Bidleman (1988) has shown that the Junge model of molecule equilibrium between the gas phase and the adsorbed phase on atmospheric particulates, represents reasonably well the fraction of adsorbed molecule as a function of their sub-cooled liquid vapour pressure. Wania and Mackay (1996) used this model to propose a classification of molecule deposition with atmospheric particulates as a function of the sub-cooled liquid vapour pressure Vpl.

Table 3: Classification from Wania and Mackay (1996)

Vpl range	Tc range °C	Expected behaviour
Vpl > 1Pa	< -50	The product stays in gaseous phase.
10^{-2} Pa <Vpl< 1Pa	-50 < < -10	High mobility, condensation and accumulation in polar phase.
10^{-4} Pa <Vpl< 10-2 Pa	-10 < < -50	Semi-mobility, condensation in mid latitudes.
Vpl < 10^{-4} Pa	>30	Low mobility, condensation near sources.

Vpl is the sub-cooled liquid vapour pressure at 25 °C.

According to this classification, compounds should stay in the gas phase if their sub-cooled vapour pressure remains higher than 1 Pa. For sub-cooled liquid vapour pressure below 10^{-4} Pa, the compound is likely to be deposited near sources.

For highly lipophilic compounds this classification applies well for 9 of the first 12 POPs (see Table 4).

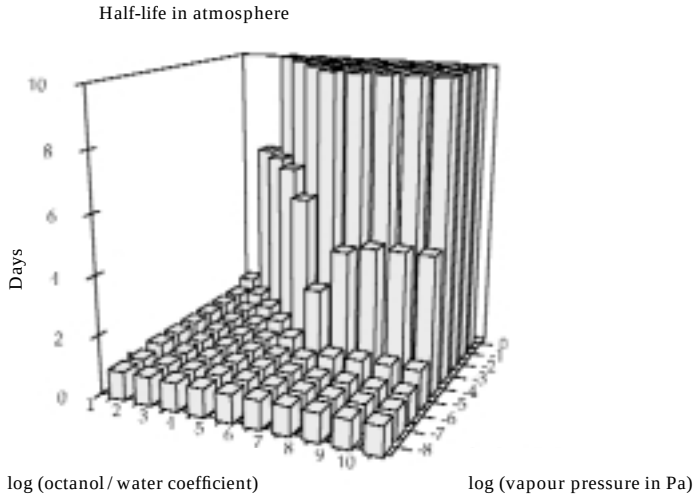
Table 4: Review of Half-lives and Vapour Pressures of 9 Chemicals Classified as POPs

Compound	Half-life in air from OH reactions	Melting point (°C)	Vapor pressure (Pa) 25°C (*20°C)	Vpl estimation (Pa)	Reference
Aldrin	2.9 h	377	0.0086	0.05	Worthing and Walker, 1983
Chlordane	1.5 d	380	0.00133	0.0086	Fram Chemicals Handbook, 1991
DDT	2.3 d	381.5	0.00002*	0.00013	Merck Index, 1983
Dieldrin	21.8 h	448	0.000103	0.003	Spencer, 1982
Endrin	21.8 h	473	0.0000266	0.0014	Callahan et al, 1979
Hexachloro benzene	2.6 y	504	0.00145*	0.16	Merck Index, 1983
Heptachlor	3.1 h	369	0.04	0.2	Budavari, 1979
Mirex	∞	758	0.00004	1.4	IARC, 1979
Toxaphene	3.2 d	363	0.0016	0.007	Wania and Mackay, 1993

Half-lives are calculated using the AOP (Kwork and Atkinson, 1995; Meylan and Howard, 1993) programme and an average concentration of OH radicals of 10^6 molecule/cm^3 (Prinn *et al*, 1995). The sub-cooled liquid vapour pressure is estimated on the basis of the simplified equation quoted by Bidleman (1988): Ln Vp/Vpl = ΔS/RT (Tm-T) with ΔSf/R ~ 6.79, where ΔSf is the fusion antropy of the compound and Tm the melting point.

This behaviour can be illustrated using the Van Pul *et al* model (1998). They presented a simple generic model for estimating the potential for long-range transboundary atmospheric transport. This note makes a simplification of their model on the basis of the following assumptions. It is a first release of the substance, so no equilibrium is expected with water, soil and sediment. The dry gas deposition velocity is modelled according to Mackay *et al* (1992). Degradation processes do not occur in any compartment. The solubility is related to the octanol-water partition coefficient according to Mackay (1982). Applying the Van Pul *et al* model with these simplifications resulted in Figure 7 which illustrates the lower limit for Vpl for a half-life in air of less than 2 days.

Figure 7



The half-life is plotted on the vertical axis. The maximum value plotted on the Z-axis is 10, but the half-lives are much longer (see Table 5). This graph shows, that the long-range transport through atmosphere of a substance with a sub-cooled liquid vapour pressure of 10^{-4} Pa and lower at ambient temperature has a very low tendency for long-range transport.

Table 5: Atmospheric Half-lives in Days as a Function of Partition Coefficient Octanol/Water (logK_{ow}) and Sub-cooled Liquid Vapour Pressure (log Vpl)

log(Vpl)	log(K_{ow})									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
0	1	7	57	392	947	1104	1123	1125	1125	1125
-1	1	1	7	57	358	771	872	884	885	885
-2	1	1	1	6	50	193	270	282	283	283
-3	1	1	1	1	6	23	35	37	37	37
-4	1	1	1	1	1	3	4	5	5	5
-5	1	1	1	1	1	1	1	1	1	1
-6	1	1	1	1	1	1	1	1	1	1
-7	1	1	1	1	1	1	1	1	1	1
-8	1	1	1	1	1	1	1	1	1	1

With respect to the half-life criteria proposed in the nomination stage with a value of 2 days, it should be noted that the adsorption on atmospheric particulates may strongly modify the rate of reaction with the atmospheric hydroxyl radical (Scheringer, 1997) and this should be taken into account in the determination of atmospheric persistence in air for example with appropriate modelling.

C.2.2 Water Transport

Recently, Wania (1999) reviewed the relative importance of transport between the different media. For low solubility compounds like DDT the flux through the atmosphere is expected to be two orders of magnitude higher than by ocean. In that case it seems justified to focus on physico-chemical properties that are significant for the atmospheric media. For higher solubility compounds fluxes of the same order may be expected in air and water. For hexachlorohexane, the ocean flux is about 5 times lower than for atmosphere.

C.3 Using multi-media modelling

Several attempts to propose transport potential calculation using modelling have been published in the literature by Van Pul *et al* (1998), Scheringer *et al* (1997) and considered during the SETAC Pellston Workshop (1999).

To take into account the effect of interaction between the different media (i.e. atmosphere, water and soil) the way of introduction into the environment and the variability of environmental conditions, multi-media modelling is the best tool. Therefore it is necessary to develop an appropriate multi-media modelling tool to assess the long-range transport capabilities of compounds.

C.4 Conclusions

Regarding the use of physico-chemical data, for highly lipophilic substances with very low water solubility like DDT, the atmosphere is most likely to be the major pathway for long-range transport. Therefore the proposals from Wania and Mackay could be applied at the nomination stage i.e. The sub-cooled liquid vapour pressure should be below 1 Pa. and higher than 10^{-4} Pa. This screening will have to be done taking into account the uncertainty on the sub-cooled liquid vapour pressure determination.

With respect to the use of multi-media models, it is essential to develop a standard tool validated by the scientific community which could be used to determine the long-range transport capabilities and deposition of molecules.

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