Institute for Health and Consumer Protection

European Chemicals Bureau

Technical Guidance Document on Risk Assessment

in support of

Commission Directive 93/67/EEC
on Risk Assessment for new notified substances

Commission Regulation (EC) No 1488/94
on Risk Assessment for existing substances

Directive 98/8/EC
of the European Parliament and of the Council
concerning the placing of biocidal products on the market

Part II

TGD

Part II

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FOREWORD

I am pleased to present this Technical Guidance Document which is the result of in-depth co-operative work carried out by experts of the Member States, the Commission Services, Industry and public interest groups. This Technical Guidance Document (TGD) supports legislation on assessment of risks of chemical substances to human health and the environment. It is based on the Technical Guidance Document in support of the Commission Directive 93/67/EEC on risk assessment for new notified substances and the Commission Regulation (EC) No. 1488/94 on risk assessment for existing substances, published in 1996. This guidance was refined taking into account the experience gained when using it for risk assessments of about 100 existing substances and hundreds of new substances. Furthermore, it has been extended to address some of the needs of the Biocidal Products Directive (Directive 98/8/EC of the European Parliament and of the Council).

Concerning Chapter 2 on Risk assessment for human health, the Exposure assessment (Assessment of workplace exposure and Consumer exposure assessment) as well as the Effects assessment were improved and refined. However, for the following sections the revision process is not yet finalised and thus, the current TGD version uses the previous text: section 2.4 on Assessment of indirect exposure via the environment and section 4 on Risk characterisation. These sections are expected to be available by the end of 2003.

With respect to Chapter 3 on Environmental risk assessment, the Environmental exposure assessment and the Effects assessment underwent major improvements. A new chapter on Marine risk assessment was added.

Concerning Chapter 7, five out of eight available Emission scenario documents (ESDs) were revised (IC-3 Chemical industry: Chemicals used in synthesis, IC-7 Leather processing industry; IC-8 Metal extraction industry, refining and processing industry; IC-10 Photographic industry; IC-13 Textiles processing industry). Furthermore, a document on Rubber industry (IC-15) and a number of ESDs for the Biocidal Product Types or parts thereof were added. Some of the Emission scenario documents are still subject to on-going consultation in the OECD and thus, may need to be revised at a later stage. In addition, ESDs to cover all 23 Biocidal Product Types are under development. Consequently, it is anticipated that the set of Emission scenario documents will be continuously expanding in the future.

The White Paper outlining a future chemicals policy was adopted in February 2001 by the Commission. This TGD is therefore to be used in support of the current legislative instruments as described above until they are revoked and replaced by the future legislation implementing the White Paper.

I hope you will agree that this TGD makes a valuable contribution to the development and harmonisation of risk assessment methodologies not only within the Community but also worldwide in the context of the activities of the Organisation of Economic Co-operation and Development and the WHO/ILO International Programme on Chemical Safety.

Ispra, April 2003

Kees van Leeuwen
Director
Institute for Health and Consumer Protection

OVERVIEW

This Technical Guidance Document is presented in four separate, easily manageable parts.

PART I

PART II

PART III

PART IV

Chapter 3

ENVIRONMENTAL RISK ASSESSMENT

CONTENTS

1 GENERAL INTRODUCTION

1.1 BACKGROUND

Directive 93/67, Regulation 1488/94 and Directive 98/8 require that an environmental risk assessment be carried out on notified new substances, on priority existing substances and active substances and substances of concern in a biocidal product, respectively. This risk assessment should proceed in the following sequence:

- hazard identification;
- dose (concentration) - response (effect) assessment;
- exposure assessment;
- risk characterisation.

The risk assessment shall be carried out for the three inland environmental compartments, i.e. aquatic environment, terrestrial environment and air, and for the marine environment.

The present document is intended to assist the competent authorities to carry out the environmental risk assessment of notified new substances, priority existing substances and active substances and substances of concern in a biocidal product. This guidance document includes advice on the following issues:

- how to calculate Predicted Environmental Concentrations (PECs) (Sections 2 and 4.2) and Predicted No-Effect-Concentrations (PNECs) (Sections 3 and 4.3) and, where this is not possible, how to make qualitative estimates of environmental concentrations and effect/no effect concentrations;
- how to conduct a PBT (persistence, bioaccumulation and toxicity) assessment (Section 4.4);
- how to judge which of the possible administrative decisions on the risk assessment according to Article 3(4) of Directive 93/67, Article 10 of Regulation 793/93 and Annex V of Regulation 1488/94 or Articles 10 and 11 of Directive 98/8 need to be taken (Section 5); and
- how to decide on the testing strategy, if further tests need to be carried out and how the results of such tests can be used to revise the PEC and/or the PNEC (Section 6).

According to Article 9(2) of Regulation 793/93, the minimum data set that must be submitted for priority existing substances is the base-set testing package required for notified new substances which is defined in Annex VIIA of Directive 67/548. This ensures that for both notified new and priority existing substances results from studies on short-term toxicity for fish, daphnia and algae are available as a minimum. Hence, the procedure for calculating PNEC as well as the testing strategy post base-set can use this as a starting point. For a new substance requirement of additional data is foreseen at level 1 and level 2 (Annex VIII of Directive 67/548). For existing substances information beyond the base-set may be available where the amount and quality of data may vary widely. For the effects assessment there may be several data available on a single endpoint, which give dissimilar results. Furthermore, there may be studies, in particular older studies, which have not been conducted according to current test guidelines and quality standards. Expert judgement will be needed to evaluate the adequacy of these data.

Directive 98/8 (Article 8, Annex IIA and Annex IIIA) stipulates data requirements for biocidal active substances. Annex IIA specifies core data requirements common to all active substances. Additional data requirements must be defined for each of 23 product types on the basis of Annex IIIA. Specification of additional data requirements takes into account the characteristics of each

product type. The common core data requirements in Annex IIA together with the specific data requirements in Annex IIIA constitute a complete set of data, adequate as a basis for risk assessment.

Due to the wide scope of the Biocidal Products Directive and the extensive variation of exposure and risks of different biocidal product types, the general rules given in the Directive and its Annexes have to be specified in order to ensure efficient and harmonised day-to-day implementation of the Directive. As written in Article 33, the Commission, in accordance with the procedure laid down in Article 28(2), shall draw up technical notes for guidance to facilitate the day-to-day implementation of this Directive.

Technical Notes for Guidance on data requirements for active substances and biocidal products (TNsG on Data Requirements, 2000; http://ecb.jrc.it/biocides/) give detailed practical guidance on choice of studies and data reporting when applying for authorisation according to Directive 98/8. It should be noted that only chemical biocidal products and substances are covered. Specific guidance is given on data requirements for substances of concern and in respect to simplified procedures, i.e. those concerning frame-formulations, low-risk biocidal products and basic substances.

Environmental exposure assessment is based on representative measured data and/or model calculations. If appropriate, available information on substances with analogous use and exposure patterns or analogous properties is taken into account. The availability of representative and reliable measured data and/or the amount and detail of the information necessary to derive realistic exposure levels by modelling, in particular at later stages in the life-cycle of a substance, will also vary. Again, expert judgement is needed.

In order to ensure that the predicted environmental concentrations are realistic, all available exposure-related information on the substance should be used. When detailed information on the use patterns, release into the environment and elimination, including information on the downstream uses of the substance is provided, the exposure assessment will be more realistic. A general rule for predicting the environmental concentration is that the best and most realistic information available should be given preference. However, it may often be useful to initially conduct an exposure assessment based on worst-case assumptions, and using default values when model calculations are applied. Such an approach can also be used in the absence of sufficiently detailed data. If the outcome of the risk characterisation based on worst-case assumptions for the exposure is that the substance is not “of concern”, the risk assessment for that substance can be stopped with regard to the compartment considered. If, in contrast, the outcome is that a substance is “of concern”, the assessment must, if possible, be refined using a more realistic exposure prediction.

The guidance has been developed mainly from the experience gained on individual organic substances. This implies that the risk assessment procedures described cannot always be applied without modifications to certain groups of substances, such as inorganic substances and metals. The methodologies that may be applied to assess the risks of metals and metal compounds, petroleum substances and ionisable substances are specifically addressed in appendices to this guidance document (Appendix VIII, IX and XI, respectively). In these appendices, it is indicated as much as possible where the text of the main document applies and where not. Where necessary, specific methods are described.

The risk assessments that have to be carried out according to Regulations 793/93 and 1488/94 for existing substances, Directives 67/548 and 93/67 for new substances and Directive 98/8 for active substances and substances of concern in a biocidal product, are in principle valid for all

countries in the European Union. It is recognised, however, that exposure estimation, for example, is subject to variation due to topographical and climatological variability. Therefore, in this document in the first stage of the exposure assessment where exposure models are used, so-called generic exposure scenarios are applied. These assume that substances are emitted into a non-existing model environment with predefined agreed environmental characteristics. These environmental characteristics can be average values or reasonable worst-case values depending on the parameter in question. Generic exposure scenarios have been defined for local emissions from a point source and for emissions into a larger region. In these generic scenarios emissions to lakes are not assessed. When more specific information on the emission of a substance is available, it may well be possible to refine the generic or site-specific assessment.

Chapter 7 (Part IV) contains for a number of use categories so-called emission scenario documents (ESDs) that give more specific information on emissions to the environmental compartments that can occur during the use of a substance. Chapter 7 includes ESDs for some types of application of biocides while scenarios describing emissions of biocides from other processes are still being developed. Such scenarios allow for quantitative emission estimation, which is an important first step in the exposure assessment, and generally has a significant influence on the outcome of risk assessments.

While comprehensive risk assessment schemes are presented for the aquatic and the terrestrial compartment and for secondary poisoning, allowing a quantitative evaluation of the risk for these compartments, the risk assessment for the air compartment can normally only be carried out qualitatively because no standardised biotic testing systems are available at present. It should also be noted that the schemes for the sediment and terrestrial compartments and for secondary poisoning are currently not supported by the same level of experience and validation as available for the aquatic compartment. These schemes will need to be further reviewed and, if necessary, revised when new scientific knowledge and experience becomes available.

The test and assessment strategies in this Technical Guidance Document are based on the current scientific knowledge and the experience of the competent authorities of the Member States. In this way, they reflect the best available scientific information to date and make use of the limited data set usually available. However, because this data set is limited, in particular for new and existing substances where the data sets are restricted to acute toxicity testing with only three trophic levels, there may be effects of substances that are not so well characterised in the assessment, such as:

- Adverse effects for which no adequate testing strategy is available yet (e.g. neurotoxicity, behavioural effects and endocrine disrupting effects);
- Specific effects in some taxa that cannot be modelled by extrapolation of the data of other taxa (for example the specific effect of organotin compounds on molluscs).

For some substances the information on the environmental release from certain stages of the life-cycle, which may include the presence of the substance in preparations, is so scarce that the PEC is quite uncertain or even not possible to estimate quantitatively. In the latter case a qualitative risk assessment is conducted (see Section 5.6).

1.2 GENERAL PRINCIPLES OF ASSESSING ENVIRONMENTAL RISKS

The environmental risk assessment approach outlined in this chapter attempts to address the concern for the potential impact of individual substances on the environment by examining both exposures resulting from discharges and/or releases of chemicals and the effects of such emissions on the structure and function of the ecosystem. Three approaches are used for this examination:

- quantitative PEC/PNEC estimation for environmental risk assessment of a substance comparing compartmental concentrations (PEC) with the concentration below which unacceptable effects on organisms will most likely not occur (predicted no effect concentration (PNEC)). This includes also an assessment of food chain accumulation and secondary poisoning;
- the qualitative procedure for the environmental risk assessment of a substance for those cases where a quantitative assessment of the exposure and/or effects is not possible;
- the PBT assessment of a substance consisting of an identification of the potential of a substance to persist in the environment, accumulate in biota and be toxic combined with an evaluation of sources and major emissions.

In principle, human beings as well as ecosystems in the aquatic, terrestrial and air compartment are to be protected. At present, the environmental risk assessment methodology has been developed for the following compartments:

For inland risk assessment:

- aquatic ecosystem (including sediment);
- terrestrial ecosystem;
- top predators;
- microorganisms in sewage treatment systems;
- atmosphere.

For marine risk assessment:

- aquatic ecosystem (including sediment);
- top predators.

In addition to the three primary environmental compartments, effects relevant to the food chain (secondary poisoning) are considered. Also effects on the microbiological activity of sewage treatment systems are considered. The latter is evaluated because proper functioning of sewage treatment plants (STPs) is important for the protection of the aquatic environment.

The methodologies implemented have as aim the identification of acceptable or unacceptable risks. This identification provides the basis for the regulatory decisions, which follow from the risk assessment. In some cases the uncertainties in carrying out the standard assessment become unacceptably high. The methodologies implemented in these cases are based on identifying the emission sources in order to identify where exposures should be minimised.

The PECs can be derived from available measured data and/or model calculations. The PNEC values are usually determined on the basis of results from single species laboratory tests or, in a few cases, established effect and/or no-effect concentrations from model ecosystem tests, taking into account adequate assessment factors. The PNEC can be derived using an assessment factor approach or, when sufficient data is available, using the statistical extrapolation methods. A

PNEC is regarded as a concentration below which an unacceptable effect will most likely not occur.

Dependent on the PEC/PNEC ratio the decision whether a substance presents a risk to organisms in the environment is taken. If it is not possible to conduct a quantitative risk assessment, either because the PEC or the PNEC or both cannot be derived, a qualitative evaluation is carried out of the risk that an adverse effect may occur.

As will be explained in more detail in the section on exposure assessment, PEC values are derived for local as well as regional situations, each of them based on a number of specific emission characteristics with respect to time and scale. As a consequence, the comparison of PNEC values for the different compartments with different PEC values for different exposure scenarios can lead to a number of PEC/PNEC ratios.

In some cases, the current quantitative risk assessment approach does not provide sufficient confidence that the environmental compartment or targets considered are sufficiently protected. The PBT assessment, given in Section 4.4, has been developed with the aim of identifying these cases.

Table 1 shows a summary of the different targets of the risk characterisation and the exposure scenarios to which they apply for inland risk assessment and **Table 2** summarises those used for the marine environment. In addition to the PECs mentioned in **Tables 1 and 2**, several other exposure levels are derived in Section 2. These are used for the assessment of indirect human exposure through the environment, which is described in Chapter 2 on Risk Assessment for Human Health. The PECs that are specifically derived for this indirect exposure assessment are summarised in **Table 3**.

Table 1 Relationship between different targets of the risk characterisation for different inland compartments

Target	Medium of exposure (PEClocal / PECregional)	Section	PNEC	Section
Aquatic organisms	Surface water	2.3.8.3 2.3.8.7	$PNEC_{water}$	3.3
Benthic organisms	Sediment	2.3.8.4 2.3.8.7	$PNEC_{sed}$	3.5
Terrestrial Organisms	Agricultural soil	2.3.8.5 2.3.8.7	$PNEC_{soil}$	3.6
Fish-eating Predators	Fish	3.8	PNECoral from $NOAEL_{avian/mammalian}$	3.8
Worm-eating Predators	Earthworms	3.8	PNECoral from $NOAEL_{avian/mammalian}$	3.8
Microorganisms	STP aeration tank	2.3.7	$PNEC_{microorganisms}$	3.4

Table 2 Relationship between different targets of the risk characterisation for different marine compartments

Target	Medium of exposure (PEClocal / PECregional)	Section	PNEC	Section
Aquatic organisms	Seawater	4.2.2 4.2.5	$PNEC_{water}$	4.3.1
Benthic organisms	Marine sediment	4.2.4.3 4.2.5	$PNEC_{marine\ sed}$	4.3.2
Fish-eating predators	Fish	4.3.3	$PNECoral_{predators}$	4.3.3
Top predators	Fish-eaters	4.3.3	PNECoral, top predators	4.3.3

Table 3 Exposure levels used for indirect human exposure

Target	Medium of exposure (PEClocal / PECregional)	Section
Drinking water production	Surface water (annual average) Groundwater	2.3.8.3 & 2.3.8.7 2.3.8.6 & 2.3.8.7
Inhalation of air	Air (annual average)	2.3.8.2
Production of crops	Agricultural soil (averaged over 180 days)	2.3.8.5 & 2.3.8.7
Production of meat and milk	Grassland (averaged over180 days)	2.3.8.5 & 2.3.8.7
Fish for human consumption	Surface water (annual average)	2.3.8.3 & 2.3.8.7

2 ENVIRONMENTAL EXPOSURE ASSESSMENT

2.1 INTRODUCTION

The environment may be exposed to chemical substances during all stages of their life-cycle from production to disposal or recovery. For each environmental compartment (air, soil, water, sediment) potentially exposed, the exposure concentrations should be derived. The assessment procedure should in principle consider the following stages of the life-cycle of a substance:

- production;
- transport and storage;
- formulation (blending and mixing of substances in preparations);
- industrial/Professional use (large scale use including processing (industry) and/or small scale use (trade));
- private or consumer use;
- service life of articles;
- waste disposal (including waste treatment, landfill and recovery).

When assessing the exposure of the environment to existing chemicals, previous releases of the chemical to the environment need to be considered. These releases may have a cumulative effect that gives rise to a "background concentration" in the environment.

Exposure may also occur from sources not directly related to the life-cycle of the substance being assessed. Examples of such sources are substances of natural origin, substances formed in combustion processes and other indirect emissions of the substance (e.g. as by-product, contaminant or degradation product of another substance). These kinds of sources have been referred to as "unintentional sources". Guidance on how to deal with emissions not covered by the life-cycle of the priority existing substance or biocidal active substance is given in Appendix XIII.

In view of uncertainty in the assessment of exposure of the environment, the exposure levels should be derived on the basis of both measured data, if available, and model calculations. Relevant measured data from substances with analogous use and exposure patterns or analogous properties, if available, should also be considered when applying model calculations. Preference should be given to adequately measured, representative exposure data where these are available (Sections 2.2.1 and 2.5).

Consideration should be given to whether the substance being assessed can be degraded, biotically or abiotically, to give stable and/or toxic degradation products. Where such degradation can occur, the assessment should give due consideration to the properties (including toxic effects) of the products that might arise. For new substances, it is unlikely that information will be available on such degradation products and thus only a qualitative assessment would normally be possible. For existing substances and biocidal active substances, however, known relevant degradation products should also be subject to risk assessment. Where no information is available, a qualitative description of the degradation pathways can be made. A summary of some of these is presented in Appendix X. Furthermore it should be noted that guidance on how to assess and test relevant metabolites and transformation products is under preparation for plant protection products under Directive 91/414. This guidance could be modified later for use for biocides, and where appropriate for new and existing substances.

For many substances available biodegradation data is restricted to aerobic conditions. However, for some compartments, e.g. sediment or ground water, anaerobic conditions should also be

considered. The same applies to anaerobic conditions in landfills and treatment of sewage sludge. Salinity and pH are examples of other environmental conditions that may influence the degradation.

In the risk assessment a proper functioning of waste treatment is assumed. However, if thermal treatment of waste is operated at insufficient technical conditions, organic substances may be formed having a PBT[1] or POP profile. This may be the case in particular in the presence of halogens (Cl and Br) and catalysing metals (e.g. copper). If the formation of PBT or POP substances is identified as a special concern, this should be noted in the risk assessment. In that case it could be considered to add an appendix to the risk assessment report with further information on the possible formation of substances with a PBT or POP profile.

2.1.1 Measured / calculated environmental concentrations

No measured environmental concentrations will normally be available for new substances. Therefore, concentrations of a substance in the environment must be estimated. In contrast, the exposure assessment of existing substances does not always depend upon modelling. Data on measured levels in various environmental compartments have been gathered for a number of existing substances. They can provide the potential for greater insight into specific steps of the exposure assessment procedure (e.g. concentration in industrial emissions, "background" concentrations in specific compartments, characterisation of distribution behaviour). The specific guidance for existing and new chemicals given below should also be applied in general for biocides.

In many cases, a range of concentrations from measured data or modelling will be obtained. This range can reflect different conditions during manufacturing and use of the substance, or may be due to assumptions in or limitations of the modelling or measurement procedures. It may seem that measurements always give more reliable results than model estimations. However, measured concentrations can have a considerable uncertainty associated with them, due to temporal and spatial variations. Both approaches complement each other in the complex interpretation and integration of the data. Therefore, the availability of adequate measured data does not imply that PEC calculations are unnecessary.

For existing substances, the rapporteur should initially make the generic "reasonable worst-case" exposure assessment based on modelling, to derive an EU environmental concentration. Measured data, i.e., site-specific or monitoring information, can then be used to revise the calculated concentrations. Other site-specific information such as effluent volumes, size of STP, river flow etc. may also be useful. In carrying out this revision, the rapporteur is recommended to include in the exposure assessment of existing substances, a table containing availability of site-specific information for each production site (if limited in number) or group of production sites (if numerous), as far as confidentiality issues allow. The "site-specific" concentrations estimated may involve the use of actual site-specific information and more generic values (and possibly extrapolated values as described below). The rapporteur should then consider in which cases extrapolation is possible from sites with site-specific information to a site without information. Aspects to consider here include the proportion of the industry covered by specific information, the nature of the industry and information about its distribution, the comparative size of sites, the types of process used etc. The rapporteur should justify in the risk assessment

[1] Substances being persistent, bioaccumulative and toxic (PBT) or substances classified as a persistent organic pollutant under the UN Stockholm Convention on Persistent Organic Pollutants.

report the grounds on which the extrapolation has been done. It may be possible to extrapolate some aspects but not others, for example emission factors (on the basis of similar processes) but not effluent flows (on the basis of differing sizes of site). If no such extrapolation can be justified, then the modelling approach described in the TGD should be followed for the (group of) site(s).

For new substances, a generic assessment would normally be conducted. However, there may be circumstances where environmental exposure for some life-cycle stages is limited to specific sites (e.g. production of chemicals, processing of intermediates etc). It may, therefore, be adequate to carry out a site-specific risk assessment only, if the Competent Authority (CA) is satisfied that such specific information will enable a full evaluation of the risks. In such cases, it is the responsibility of the notifier to provide site-specific data and to show that the available information is valid for the sites being assessed. The risk assessment should make clear that a site-specific assessment has been conducted. In these cases, the notifier is obliged to confirm in writing that they will inform the CA of any relevant changes, which may affect the risk assessment conducted. The CA should confirm details of the assessment not later than two years after completion of the risk assessment, and at any subsequent tonnage trigger, or as deemed necessary. The CA should distribute relevant information appropriately.

It should be noted that the site-specific risk assessment is not based on a detailed and complete description of the environmental conditions. The aim is to estimate environmental concentrations that are reasonably applicable for a European-level risk assessment. Some site-specific data may be used to replace the default data characterising the standard scenario.

For measured data, the reliability of the available data has to be assessed as a first step. Subsequently, it must be established how representative the data are of the general emission situation. Section 2.2 provides guidance on how to perform this critical evaluation of measured data. For model calculations, the procedure to derive an exposure level should be made transparent. The parameters and default values used for the calculations must be documented. If different models are available to describe an exposure situation, the best model for the specific substance and scenario should be used and the choice should be explained. If a model is chosen which is not described in this document, that model should be explained and the choice justified. Section 2.3 discusses modelling in detail. Section 2.5 gives further advice on critical comparison between calculated and measured PECs.

2.1.2 Relationship between PEClocal and PECregional

For the release estimation of substances, a distinction is usually made between substances that are emitted through point sources at specific locations and substances that enter the environment through diffuse releases. Point source releases have a major impact on the environmental concentration on a local scale (PEClocal) and also contribute to the environmental concentrations on a larger scale (PECregional).

When determining a PEC for new substances at base-set level, or at the 10 tonnes per annum production level, Annex III, paragraph 3.4 of Directive 93/67 foresees that such estimates will usually focus on the generic local environment to which releases may occur. In the case of persistent and/or highly toxic chemicals, however, a regional assessment may still be relevant at low tonnages. Therefore, derivation of a PECregional is required, unless it can be justified that a regional assessment is not relevant for the substance at these low tonnages.

PEClocal

The concentrations of substances released from point sources are assessed for a generic local environment. This is not an actual site, but a hypothetical site with predefined, agreed environmental characteristics, the so-called "standard environment". These environmental conditions can be average values, or reasonable worst-case values, depending on the parameter in question. The scale is usually small and it is assumed that the targets are exposed in, or at the border of, the area. In general, concentrations during an emission episode are measured or calculated. This means that PEClocal is calculated on the basis of a daily release rate, regardless of whether the discharge is intermittent or continuous. It represents the concentration expected at a certain distance from the source on a day when discharge occurs. Only for the soil compartment (being a less dynamic environment than air or surface water) longer-term averages apply. However, in some cases time related concentrations may be obtained, for instance in situations where intermittent releases occur. In principle, degradation and distribution processes are taken into consideration for the PEClocal. However, because of the relatively small spatial scale, only one or two key processes typically govern the ultimate concentration in a compartment.

PECregional

The concentrations of substances released from point and diffuse sources over a wider area are assessed for a generic regional environment. The PECregional takes into account the further distribution and fate of the chemical upon release. It also provides a background concentration to be incorporated in the calculation of the PEClocal. As with the local models, a generic standard environment is defined. The PECregional is assumed to be a steady-state concentration of the substance.

Concentrations in air and water are also estimated at a continental scale (Europe) to provide inflow concentrations for the regional environment. These concentrations are not used as endpoints for exposure in the risk characterisation.

Figure 1 illustrates the relationships between the three spatial scales. The local scale receives the background concentration from the regional scale; the regional scale receives the inflowing air and water from the continental scale.

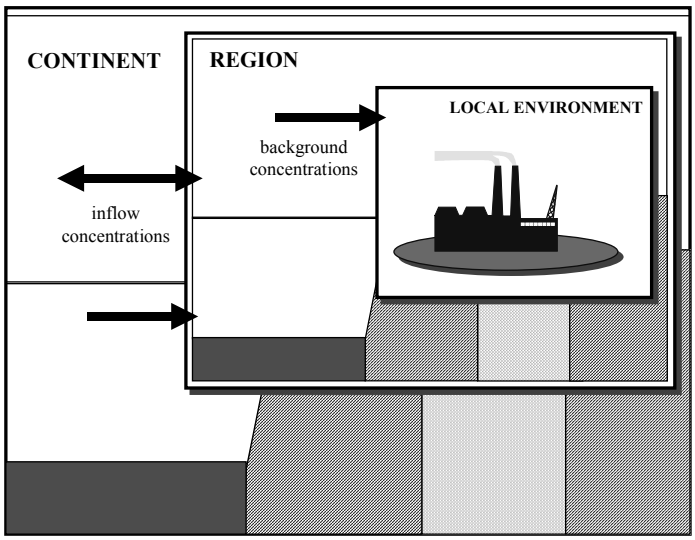

Figure 1 The relationship between the continental, regional, and local scale exposure assessments

This implies that the continental, regional, and local calculations must be done sequentially. It should be noted that the use of regional data as background for the local situation may not always be appropriate. If there is only one source of the substance, this emission is counted twice at the local scale: not only due to the local emission, but the same emission is also responsible for the background concentration of the region.

2.2 MEASURED DATA

For a number of existing substances measured data are available for air, fresh or saline water, sediment, biota and/or soil. These data have to be carefully evaluated for their adequacy and representativeness according to the criteria below. They are used together with calculated environmental concentrations in the interpretation of exposure data.

The evaluation should follow a stepwise procedure:

- reliable and representative data should be selected by evaluation of the sampling and analytical methods employed and the geographic and time scales of the measurement campaigns (Section 2.2.1);
- the data should be assigned to local or regional scenarios by taking into account the sources of exposure and the environmental fate of the substance (Section 2.2.2);
- the measured data should be compared to the corresponding calculated PEC. For naturally occurring substances background concentrations have to be taken into account. For risk characterisation, a representative PEC should be decided upon based on measured data and a calculated PEC (Section 2.5).

2.2.1 Selection of adequate measured data

The available measured environmental concentrations have to be assessed first. The following aspects could be considered in order to decide if the data are adequate for use in the exposure assessment and how much importance should be attached to them:

Quality of the applied measuring techniques

The applied techniques of sampling, sample shipping and storage, sample preparation for analysis and analysis must consider the physico-chemical properties of the substance. Measured concentrations that are not representative as indicated by an adequate sampling programme or are of insufficient quality should not be used in the exposure assessment.

The limit of quantitation (LOQ) of the analytical method, which is normally defined by the analytical technique being used, should be suitable for the risk assessment and the comparability of the measured data should be carefully evaluated. For example, the concentrations in water may either reflect total concentrations or dissolved concentrations according to the sampling and preparation procedures used. The concentrations in sediment may significantly depend on the content of organic carbon and particle size of the sampled sediment. The soil and sediment concentrations should preferably be based on concentrations normalised for the particle size (i.e. coarsest particles taken out by sieving). All measurements below the LOQ constitute a special problem and should be considered on a case-by-case basis. One approach that could be considered would be to use a value corresponding to LOQ/2 before estimating a mean or standard deviation (EC, 1999). As this method could heavily influence the mean and standard deviation, other methods may also be considered (e.g. assuming same distribution of data below and above the LOQ).

The aim is to obtain as much useful information on exposure from a data set as possible, but there is inherent danger for inappropriate use of the data for risk assessment purposes. To address this problem, two quality levels for existing data are given in **Table 4** (taken from OECD, 2000k). In recommending this table the OECD stressed "…these criteria should be applied in a flexible manner. For example, data should not always be discounted because they do not meet the criteria. Risk assessors should make a decision to use the data or not, on a case-by-

case basis, according to their experience and expertise and the needs of the risk assessment". The most important factors to be addressed are the analytical quality control and the representativeness of the sample. Clearly at concentrations approaching the LOQ of an analytical method, percentage errors will be greater than at higher concentrations.

Table 4 Quality criteria for use of existing data (OECD, 2000k)

Study category		
	1	**2**
Criteria	Valid without restriction – may be used for measured PEC	Valid with restrictions - May be used to support Exposure Assessment (data interpretation difficult)
What has been analysed? 1)	x	x
Analytical method 2)	x	x
Unit specified 3)	x	x
Limit of quantitation 4)	x	x
Blank concentration 5)	x	
Recovery 6)	x	
Accuracy 7)	x	
Reproducibility 8)	x	
Sample collection 9)	x	
One shot or mean 10)	x	x
Location 11)	x	x
Date dd/mm/yy 12)	x	Minimum is knowledge of year
Compartment characteristics 13)	x	
Sampling frequency and pattern	x	x
Proximity of discharge points 14)	x	x
Discharge emission pattern and volume 15)	x (for local scale)	x (for local scale)
Flow and dilution or application rate	x (for local scale)	x (for local scale)
Explanation of value assigned to non-detects if used in a mean	x	x

Notes to Table 4:

1) Precisely what has been analysed should be made clear. Details of the sample preparation, including for example whether the analysis was of the dissolved fraction, the suspended matter (i.e. adsorbed fraction) or the total (aqueous and adsorbed) should be given.
2) The analytical method should be given in detail or an appropriate reference cited (e.g. the relevant ISO/DIN method or standard operating procedure).
3) Units must be clearly specified and information given whether it has been normalised to e.g. organic carbon, lipid etc.
4) The limit of quantitation and details of possible known interfering substances should be quoted.
5) Concentrations in system blanks should be given.
6) Recovery of standard additions (spikes) should be quoted.
7) Results of analysis of standard "reference samples", containing a known quantity of the substance should be included. Accuracy is connected to the analytical method and the matrix.
8) The degree of confidence (e.g. 95% confidence interval) and standard deviation in the result from repeat analysis should be given. Reproducibility is also connected to the analytical method and the matrix.
9) Whether the sampling frequency and pattern relate to the emission pattern, or whether they allow for effects such as seasonal variations need to be considered.
10) The assessor needs to know how the data have been treated, e.g. are the values reported single values, means, 90-percentile, etc.
11) The monitoring site should be representative of the location and scenario chosen. If data represent temporal means, the time over

which concentrations were averaged should be given too.

12) The time, day, month and year may all be important depending upon the release pattern of the chemicals. Time of sampling may be essential for certain discharge/emission patterns and locations. For some modelling and trends analysis, the year of sampling will be the minimum requirements.
13) Compartment characteristics such as lipid content, content of organic carbon and particle size should be specified.
14) For the local aqueous environment, detailed information on the distance of other sources in addition to quantitative information on flow and dilution are needed.
15) It is necessary to consider whether there is a constant and continuous discharge, or whether the chemical under study is released as a discontinuous emission showing variations in both volume and concentration with time.

When a substance is used in materials (e.g. polymers) it may be released to the environment enclosed within the matrix of small particles of the material formed e.g. by weathering or abrasion (see 2.3.3.5). In such cases it would be useful to know if the analytical method used is able to detect also the fraction of substance that is associated with these particles. The availability for analysis can be expected to be reduced for resistant materials and/or large particles. Depending on use pattern, particles may end up in STP sludge/agricultural soil, sediments affected by storm water outflows, industrial/urban soil and indoor dust.

Selection of representative data for the environmental compartment of concern

There are two distinct aspects to consider:

The level of confidence in the result, i.e. the number of samples, how far apart and how frequently they were taken. The sampling frequency and pattern should be sufficient to adequately represent the concentration at the selected site.

Whether the sampling site(s) represent a local or regional scenario. Samples taken at sites directly influenced by an emission should be used to describe the local scenario, while samples taken at larger distances may represent the regional concentrations.

It has to be ascertained if the data are results of sporadic examinations or if the substance was detected at the same site over a certain period of time. Measured concentrations caused by an accidental spillage or malfunction should not be considered in the exposure assessment.

Where outliers have been identified their inclusion/exclusion should be discussed and justified. The data should be critically examined to establish whether high values reflect an increased or new release, a recent change in emission pattern or a newly discovered occurrence in a specific environmental compartment. The data should also be examined to check that the analytical methodology was appropriate.

If many data are available, the following statistical approach for defining outliers may be used:

$$\log(X_i) > \log(p_{75}) + K(\log(p_{75}) - \log(p_{25})) \quad (1)$$

Where X_i is the concentration, above which a measured value may be considered an outlier, p_i is the value of the i^{th} percentile of the statistic and K is a scaling factor. This filtering of data with a scaling K = 1.5 is used in most statistical packages, but this factor can be subject dependent.

Data from a prolonged monitoring programme, where seasonal fluctuations are already included, are of special interest. If available, the distribution of the measured data could be considered for each monitored site, to allow all the information in the distribution function to be used. For regional PEC assessment, a further distribution function covering several sites could be constructed from single site statistics (for example, median, or 90^{th} percentile if the distribution

function has only one mode), and the required 90th percentile values, mean or median values of this distribution could be used in the PEC prediction. The mean of the 90th percentiles of the individual sites within one region is recommended for regional PEC determination. Care should be taken that data from several sites obtained with different sampling frequencies should not be combined, without appropriate consideration of the number of data available from each site. If individual measurements are not available then results expressed as means and giving standard deviation will be of particular relevance because in most instances a log normal distribution of concentrations can be assumed and a 90th percentile concentration may be calculated. If only maximum concentrations are reported, they should be considered as a worst-case assumption, providing they do not correspond to an accident or spillage. However, use of only the mean concentrations can result in an underestimation of the existing risk, because temporal and/or spatial average concentrations do not reflect periods and/or locations of high exposure.

For intermittent release scenarios, even the 90-percentile values may not properly address emission episodes of short duration but of high concentration discharge. In these cases, mainly for PEClocal calculations, a more realistic picture of the emission pattern can be obtained from the highest value of average concentrations during emission episodes.

Representative measured data from monitoring programmes or from literature, for comparison with calculated PECs should be compiled as tables and annexed to the risk assessment report. The measured data should be presented in the following manner:

Location	Substance	Concentration	Period	Remark	Reference
Country – location	substance or metabolite	Units: [µg/L], [ng/L] [mg/kg], etc Data - mean - average - range - percentile - daily - weekly - monthly - annual - etc	month, year	limit of quantitation (LOQ) relevant information on analytical method analytical quality control	Literature reference

When emissions of a substance from waste treatment or disposal stages are significant, measured data may be important along with model calculations in the assessment of the release of the substance from the waste life stage. Besides measured data on concentrations in leachate and landfill gases it is important that flows of water and, when appropriate, gases and solids, from principal treatment or disposal processes and facilities are measured (see Sections 2.3.3.6 and 2.3.7.2) to obtain flow-weighted concentrations. As a surrogate and complement, average time trend data on real runoff or landfill gas production data can be used, also to extend flux measures to long-term estimates. Emission data of higher quality may become available when the European Pollutant Emissions Register is fully implemented.

However, for release scenarios from waste disposal operations including landfills, the measured concentration may underestimate the environmental concentration that might occur once a substance has passed through all the life-cycle stages including the possible delays (see Section 2.3.3.6). In selecting representative data for waste related releases, consideration should be given to the question whether or not production/import of the substance is in steady state with the

occurrence of substance in the waste streams and/or releases from waste treatment and/or releases from landfills.

In a similar manner, if the amount of a substance in use in the society in long-life articles has not reached steady state and the accumulation is ongoing, only a calculated PEC will represent the future situation. This should be considered when comparing such a PEC with measured data representing a non-steady-state.

For the evaluation of measured concentration in biota additional information on season, sex and dimension could be useful.

2.2.2 Allocation of the measured data to a local or a regional scale

The measured data should be allocated to a local or regional scale in order to define the nature of the environmental concentration that is derived. This allows a comparison with the corresponding calculated PEC to be made to determine which PEC should be used in the risk characterisation (Section 2.5).

Evaluation of the geographical relation between emission sources and sampling site

If there is no spatial proximity between the sampling site and point sources of emission (e.g. from rural regions), the data represent a regional concentration (PECregional) that has to be added to the calculated PEClocal. If the measured concentrations reflect the releases into the environment through point sources, they are of a PEClocal-type. In a PEClocal based on measured concentrations, the regional concentration (i.e. PECregional) is already included.

Measured concentrations in biota

Samples of living organisms may be used for environmental monitoring. They can provide a number of advantages compared to conventional water and sediment sampling especially with respect to sampling at large distances from an emission source or on a regional scale. Furthermore they can provide a PEC_{biota} and consequently an estimation of the body burden to be considered in the food chain.

2.3 MODEL CALCULATIONS

2.3.1 Introduction

The first step in the calculation of the PEC is evaluation of the primary data. The subsequent step is to estimate the substance's release rate based upon its use pattern. All potential emission sources need to be analysed, and the releases and the receiving environmental compartment(s) identified. After assessing releases, the fate of the substance once released to the environment needs to be considered. This is estimated by considering likely routes of exposure and biotic and abiotic transformation processes. Furthermore, secondary data (e.g. partition coefficients) are derived from primary data. The quantification of distribution and degradation of the substance (as a function of time and space) leads to an estimate of PEClocal and PECregional. The PEC calculation is not restricted to the primary compartments; surface water (Section 2.3.8.3), soil (Section 2.3.8.5) and air (Section 2.3.8.2); but also includes secondary compartments such as

sediments (Section 2.3.8.4) and groundwater (Section 2.3.8.6). Transport of the substance between the compartments must, where possible, be taken into account.

This section is arranged as follows:

- description of the minimum data set requirements for the distribution models described in the following sections;
- estimation of releases to the environment;
- definition of the characteristics of the standard environment used in the estimation of PECs on the local and regional scale;
- derivation of secondary data: intermedia partition coefficients and degradation rates. These parameters might be part of the data set, otherwise, they are derived from primary data by estimation routines;
- fate of the substance in sewage treatment;
- fate of substances in waste incineration, landfills and/or recovery operations;
- distribution and fate in the environment, and estimation of PECs (local and regional).

The structure of this section is shown schematically in **Figure 2**, including the flow of data between the separate steps of the calculations.

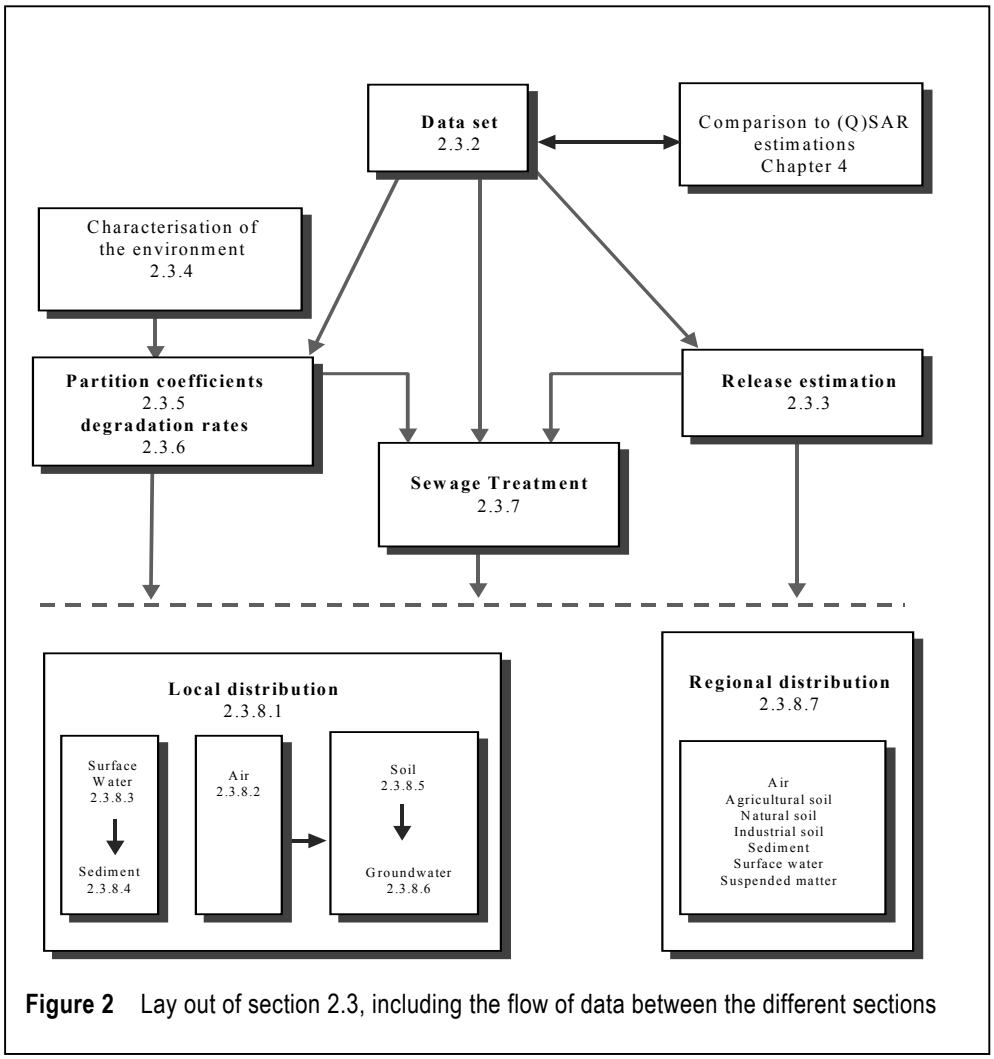

Figure 2 Lay out of section 2.3, including the flow of data between the different sections

The model calculations are given in each section. The following table format is used for explaining the symbols used in an equation:

Explanation of symbols

[Symbol]	[Description of required parameter]	[Unit]	[Default value, equation number where this parameter is calculated, or
[Symbol]	[Description of resulting parameter]	[Unit]	reference to a table with defaults]

The following conventions are applied where possible for the symbols

- parameters are mainly denoted in capitals;
- specification of the *parameter* is done in lower case;
- specification of the *compartment* for which the parameter is specified is shown in subscripts.

Some frequently occurring symbols

E	for emissions (direct and indirect)	$[kg \cdot d^{-1}]$
F	for dimensionless fractions	$[kg \cdot kg^{-1}]$ or $[m^3 \cdot m^{-3}]$
C	for the concentration of a substance	$[mg \cdot l^{-1}]$, $[mg \cdot kg^{-1}]$ or $[mg \cdot m^{-3}]$
RHO	for densities of compartments or phases	$[kg \cdot m^{-3}]$
K	for intermedia partitioning coefficients	[various units apply]
k	for (pseudo) first-order rate constants	$[d^{-1}]$
T	for a period of time	[d]

As an example, the symbol Foc_{soil} means the fraction (*F*) organic carbon (*oc*) in the soil compartment (*soil*). For other parameters, recognisable symbols are chosen. It should be noted that in several equations fixed factors (e.g. 1000 or 10^6) are applied for dimensional consistency.

Sensitivity analysis

In the case of conflicting data, great variation or uncertainty in data, a few carefully selected scenarios could be considered employing alternative input parameters for the fate-related properties in question. The fate-related properties may include data for bioaccumulation, sorption, degradation, volatilisation etc. The concept may also be useful for emissions if they are uncertain in relation to their size to certain environmental compartments.

However “the best value” according to the “realistic worst case” should be used in the “core assessment”, and the alternative input values should only be included in alternative estimations performed for investigation purposes. It should be noted that fixing a parameter, which results in e.g. a higher PEC/PNEC ratio for sediment, soil, secondary poisoning and STP, will result in a lower PEC/PNEC ratio for pelagic organisms. Therefore, in such cases it is possible that one particular set of parameters will give rise to the highest risk for one compartment, and another set for another compartment; both might be valid extremes.

The approach described above should especially be considered in relation to multi-component substances / groups of substances where the intrinsic properties vary between the different components of the substance. It is important to know which components any measured values relate to. The concept may, however, also be useful for certain discrete substances, where there is special uncertainty about a fate related property or an emission that may be of key importance.

The outcome of the alternative exposure assessments should be presented in an illustrative appendix to the risk assessment report. If the analysis shows that the variation of the input parameter(s) is critical in relation to the result of the assessment (i.e. changes the conclusion), then further consideration is necessary of ways to improve the certainty of the input parameter(s) in question. If on the other hand the analysis shows that the results of the assessment are not changed, the confidence in the assessment has increased.

2.3.2 Data for exposure models

The following parameters from the base-set are directly used in the exposure models as discussed in the following sections:

Physico-chemical properties

MOLW	molecular weight	[g · mol^{-1}]
Kow [2]	octanol water partitioning coefficient	[-]
SOL	water solubility	[mg · l^{-1}]
VP	vapour pressure	[Pa]
BOILPT	boiling point (only for some release estimations)	[°C]

Use pattern of the substance

PRODVOL	production volume of substance	[tonnes · yr^{-1}]
IMPORT	volume of substance imported	[tonnes · yr^{-1}]
EXPORT	volume of substance exported	[tonnes · yr^{-1}]
INDCAT	industrial category	[-]
USECAT	use category	[-]
MAINCAT	main category (for existing substances)	[-]
Specific information on the use pattern of the substance		

Sections 2.3.5 and 2.3.6 describe how secondary data (partition coefficients and degradation rates) are derived from the minimum data requirements. When adequately measured data are known, these should be used instead of the estimations.

It should be noted that the data requirements for the exposure models, as listed above, are only valid for neutral, organic, non-ionised substances. Before proceeding with the modelling exercise due consideration should be given whether the substance can be classified as a neutral, organic, non-ionised substance. More specific information (e.g. partition coefficients or pKa/pKb for ionising substances) may be required for other types of substances. For ionising substances, the pH-dependence of Kow and water solubility should be known. Partition coefficients should be corrected according to the pH of the environment (see Appendix XI).

For surface active substances it may not be advisable to use estimated or measured Kow values as a predictor for e.g. Koc (soil, sediment, suspended organic matter and sludge) and BCF (fish, worm) because the predictive value of log Kow for such estimations may be too low. Instead, for surfactants it may be appropriate to obtain measured Kp and BCF values.

If experimentally determined physico-chemical data have been obtained at a temperature which for the substance under consideration would significantly change when extrapolated to the

[2] The term Kow is used in this document and is equivalent to Pow.

relevant temperature of the exposure models employed (e.g. 12°C in the regional model) then such an extrapolation should be considered. In most cases this will not be necessary.

However, the vapour pressure may for some substances change considerably according to the temperature even within a temperature range of only 10°C. In this case a general temperature correction should be applied according to the following equation:

$$VP(TEMP_{env}) = VP(TEMP_{test}) \cdot e^{\left(\frac{H_{0vapor}}{R} \cdot \left(\frac{1}{TEMP_{test}} - \frac{1}{TEMP_{env}}\right)\right)} \quad (2)$$

Explanation of symbols

$VP(TEMP_{env})$	vapour pressure at the environmental temperature	[Pa]	
$VP(TEMP_{test})$	vapour pressure as give in the data set	[Pa]	data set
$TEMP_{env}$	environmental temperature (scale-dependent)	[K]	
$TEMP_{test}$	temperature of the measured experimental VP	[K]	
H_{0vapor}	enthalpy of vapourisation	[J/mol]	$5 \cdot 10^4$
R	gas constant	[Pa · m³/(mol · K)]	8.314

Care must be taken when the melting point is within the extrapolated temperature range. The vapour pressure of the solid phase is always lower than the extrapolated vapour pressure of the liquid phase. Extrapolation will therefore tend to overestimate the vapour pressure. There is no general solution to this problem.

The same approach can be followed for correcting the water solubility:

$$SOL(TEMP_{env}) = SOL(TEMP_{test}) \cdot e^{\left(\frac{H_{0solut}}{R} \cdot \left(\frac{1}{TEMP_{test}} - \frac{1}{TEMP_{env}}\right)\right)} \quad (3)$$

Explanation of symbols

$SOL(TEMP_{env})$	solubility at the environmental temperature	[Pa]	
$SOL(TEMP_{test})$	solubility as give in the data set	[Pa]	data set
$TEMP_{env}$	environmental temperature (scale-dependent)	[K]	
$TEMP_{test}$	temperature of the measured experimental SOL	[K]	
H_{0solut}	enthalpy of solution	[J/mol]	$1 \cdot 10^4$
R	gas constant	[Pa · m³/(mol · K)]	8.314

2.3.3 Release estimation

In this section the following parameters are derived:

- local emission, the rates to air and waste during an emission episode;
- regional emissions to air, wastewater, and industrial soil (annual averages).

2.3.3.1 Life-cycle of substances

Releases into the environment can take place from processes at any stage of the life-cycle of a substance (**Figure 3**). The stages are discussed briefly below.

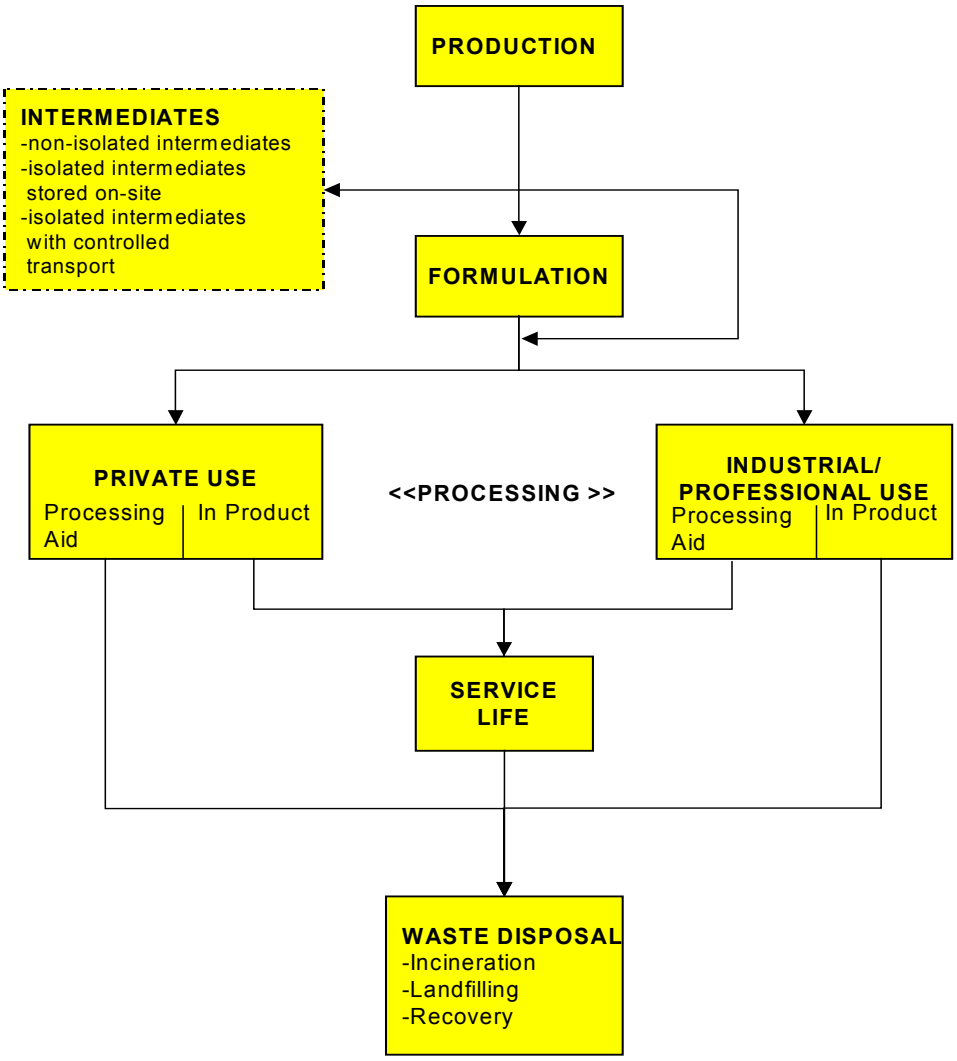

Figure 3 Schematic representation of the life-cycle of a substance

Production

Production is the stage where the substance is manufactured, i.e. formed by chemical reaction(s), isolated, purified, drummed or bagged, etc. For intermediates (chemicals used to make other chemicals) a distinction is made between non-isolated, site-limited, and captive intermediates, as shown in **Figure 3**.

- Non-isolated intermediates: the substance is not isolated from the reaction mixture but transformed directly into another substance in the same equipment in a subsequent reaction step;
- Site-limited intermediates: the substance is manufactured and consumed at the same site. This signifies that releases at production and industrial/professional use (the transformation into the next substance) occur at the same site;
- Captive intermediates: the intermediate is manufactured and shipped to other sites owned by the same company, but not sold to others. Therefore, releases at production of captive and other intermediates occur at another site where the substance is transformed into the next substance.

Transport and storage

Guidance is currently not included for the estimation of emissions during transport and storage.

Formulation

Formulation is the stage where substances are combined in a process of blending and mixing to obtain a product or a preparation. This may be a formulation such as a paint, or a product such as a photographic film. Formulations are applied or used at the next stages of the life-cycle (industrial/professional use, private use).

Industrial/professional use

The stage of industrial/professional use consists of all kinds of processes where the substance as such, a formulation, or an article containing the substance assessed, is applied or used. A substance produced at one site may be used as intermediate at other sites in the manufacture of other substances. Substances may be used as a processing aid or be incorporated in a product. One example of a processing aid is a developer used in a photographic bath that is disposed of after use. It should be noted that the manufacture of photographic film and paper might also be considered as processing of the substances involved. Industrial/professional use can take place at variable scale, including single and multiple sites.

Private use

This stage considers the use and application of substances as such (or in formulations such as cosmetics and biocides) at the scale of households (consumers).

Service life

Articles like a plastic cable or articles with a coating layer containing the assessed substance will be used over a certain period of time. Releases into the environment during this period due to migration, leaching, evaporation and processes such as weathering and abrasion are calculated separately (see Section 2.3.3.5).

Waste disposal (including waste treatment and recovery)

At the end of the service life, the substance or a product containing the substance enters into the waste disposal stage with waste or wastewater (**Figure 4).** Waste treatment may include incineration or removal to landfill.

At this stage recovery processes may be applied. These usually involve a homogenisation and/or separation step (e.g. mechanical treatment) followed by recovery of the target substance/material. The recovered substance or material may be:

- reprocessed for the original type of product (recycling);
- manufactured into a new type of product;
- used as secondary fuel in heat production.

In the first option the substance returns into life-cycle stages already assessed before. In the second and third option the substance may enter into processing and final products from which new types and amounts of releases could occur. Whether or not these releases could be relevant to consider a case-by-case assessment. Some general criteria are given in Section 2.3.7.2.

In some cases, another substance or product may be recycled, and the substance assessed is present in this product. Releases in this situation may vary widely and information on them may not be readily available since the focus of attention is not on the substance assessed, but on the substance or product recovered.

A substance present in a photographic bath for example, will be released at discharge after silver recovery, and a substance present in printing ink will be released with wastewater and de-inking sludge at paper recycling.

Releases from prolonged use of a product or articles in new applications after first service life (e.g. tyres in agriculture) without a waste specific treatment step in between should be assessed as a separate use in the relevant life-cycle stages i.e. processing/service, as appropriate.

In addition to being incinerated or being disposed of in landfill, waste may be released, either intentionally or unintentionally, to the environment. Articles may intentionally be left in the environment after their service life (e.g. cables buried in soil). Demolished building materials may be used as ballast at e.g. road constructions. Fragments of articles may also be lost during use (e.g. paint flakes, car undercoating).

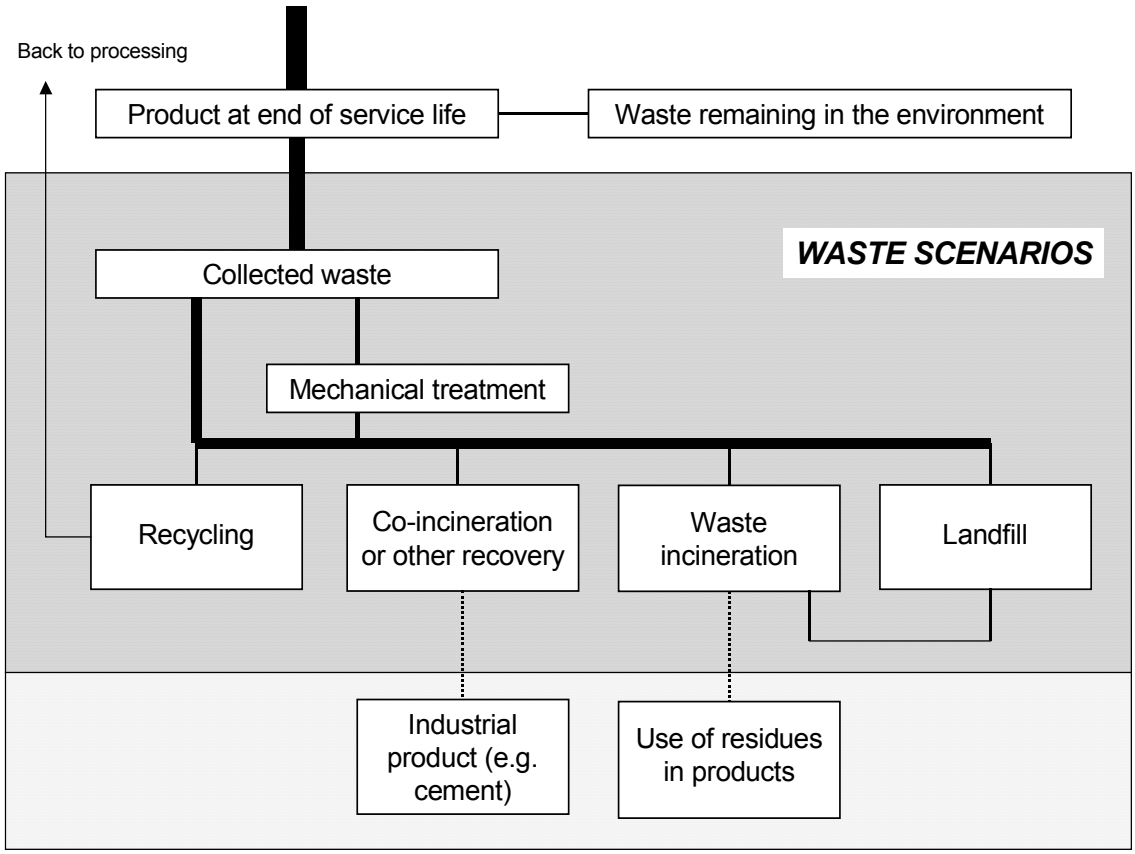

Figure 4 Schematic representation of the waste life stage of a substance

2.3.3.2 Types of emissions and sources

Emission patterns vary widely from well-defined point sources (single or multiple) to diffuse releases from large numbers of small point sources (like households) or line sources (like a motorway with traffic emissions). Releases may also be continuous or intermittent. Continuous emissions are characterised by an almost constant emission rate flow over a prolonged period (e.g. the emission of a substance from a continuous production process such as an oil refinery). Intermittent emissions can be peak emissions or block emissions (see Section 2.3.3.4). Peak emissions are characterised by a relatively large amount discharged in a short time where the time intervals between peaks and the peak height can vary greatly (e.g. the discharge of spent liquid - reaction mixture - after isolation of the synthesised substance in a batch process). Block emissions are characterised by a flow rate which is reasonably constant over certain time periods with regular intervals with a low or even zero background emission (e.g. the emissions from traffic during the day; during rush hours emission are particularly high). The quantities released from a certain process may vary from 100%, as is the case for example with household products like detergents or volatile solvents in paints, to below 1% for substances like intermediates produced in closed systems.

Besides releases from point sources, diffuse emissions from articles during their service life may contribute to the total exposure for a substance. For substances used in long-life materials this may be a major source of emissions (both during use and as waste remaining in the environment, see Section 2.3.3.5).

Emissions related to the waste life stage can take place several decades after production and processing of a substance. They may follow the market volume of the substance with a delay specific for a certain type of product. Emission patterns (e.g. route, quantity and trend in time) may also be determined by the type of treatment in relation to substance properties. Little is known of the magnitude of long-term releases, e.g. of metals or of organic substances that do not degrade anaerobically (see Section 2.3.3.6).

2.3.3.3 Release estimation

It is clear that the releases of a substance are dependent on the use patterns. Three categories are distinguished, i.e. main category, industry category and function or use category. An overview of these categories can be found in Chapter 5. The main categories are intended to describe generally the exposure relevance of the use(s) of a substance. In the context of environmental risk assessment they are also used to characterise release scenarios for the estimation of emissions to the environment during specific stages of the life-cycle of the substance (production, formulation, and industrial/professional use). They can therefore be allocated to release fractions, which are used as default values where specific information is missing. The following Main Categories are distinguished:

- use in closed systems: refers to the industrial/professional use stage when a substance is used for example in a transformer or a circulation circuit of a refrigerator, or it may refer to the stage of production where a substance like an intermediate is manufactured in closed apparatus;
- use resulting in inclusion into or onto a matrix: refers to the stage of formulation, e.g. when a substance is included in the emulsion layer of a photographic film. It also may refer to the stage of industrial/professional use, e.g. when a substance, applied as a uv-stabiliser in paint, ends up in the finished coating layer;
- non-dispersive use: relates to the number (and size) of the emission sources;
- wide dispersive use: relates also to the number (and size) of the emission sources.

The industry categories specify the branch of industry (including personal and domestic use, and use in the public domain) where considerable emissions occur by application of the substance as such, or by the application and use of preparations and products containing the substance. Some important emission sources have not been included specifically in this scheme and hence have to be allocated to category “Others” (no. 15/0), e.g. emissions of substances (in preparations) other than fuels and fuel additives used in motor vehicles.

The use or function category specifies the specific function of the substance. There are 55 categories which have a varying level of detail. For substances used in photography for example, there is only one category: 42 “Photochemicals”. Depending on the specific function of the photochemical, however, emissions can vary to a great extent, e.g. substances used to influence the crystal growth of silver compounds at the production of films are released by over 50%, while other substances at this stage will hardly be released. There is no general category as “Plastics additives” and many other specific categories lack as well; exceptions are categories like 47 “Softeners” (= plasticisers) and 49 “Stabilisers” (heat and UV-stabilisers).

The release of a substance at different stages of its life-cycle should be estimated by order of preference from:

1. specific information for the given substance (e.g. from producers, product registers or open literature);
2. specific information from the emission scenario documents (use category documents) for several industrial categories as well as for some of the 23 biocidal Product Types as given in Part IV, Chapter 7;
3. emission factors as included in the release tables of Appendix I.

Emissions may occur from a category other than the one to which a substance is allocated. A substance used in paint will normally be allocated to category 14 “Paints, lacquers and varnishes”. Though the local emissions of solvents may be considerable at one point source (the paint factory) at the stage of formulation (paint production), most of the solvent will be emitted at paint application. The application could be classified in several industrial categories depending on the type of paint. In case of a do-it-yourself paint it would belong to category 5 “Personal/domestic”, in case of motor car repair or professional house painting it would be category 15/0 “Others” (wide dispersive use, so diffuse releases) and in case of motor car production 16 “Engineering industry: civil and mechanical” (non-dispersive use, so few large point sources).

It is possible that confusion arises when the use of a substance, belonging to a certain specific process of an industrial category, occurs at another branch of industry. One example is the application of an additive for an epoxy resin applied in the electronic industry for the embedding of electronic components. Though the industrial/professional use takes place at category 4 “Electrical/electronic engineering industry” the industrial/professional use of epoxy resins belongs to category 11 “Polymers industry”. The releases from the process will be found in the table for the latter category. Further information on main categories, industry categories and use categories is provided in Appendix I, together with more examples.

For chemical industry, two separate industrial categories exist, one for basic chemicals and another for chemicals used in synthesis. Basic chemicals are considered to comprise commonly used chemicals such as solvents and pH-regulating agents such as acids and alkalis. Also the primary chemicals from the oil refining process are considered as basic chemicals. Substances used in synthesis fall in two classes, namely intermediates (substances produced from a starting material to be converted in a subsequent reaction into a next substance) and other substances. These other substances consist mainly of 'process regulators' (e.g. accelerators, inhibitors, indicators). For industrial category 5 (personal/domestic) the use and application of substances (as such or in formulations) is considered at the scale of households. The types of application are e.g. adhesives, cosmetics, detergents, and pharmaceuticals. Some applications have been covered in other industrial categories at the stage of private use. These applications comprise fuels and fuel additives (mineral oil and fuel industry), paint products (paints, lacquers and varnishes industry) and photochemicals (photographic industry). For industrial category 6 (public domain), use and application at public buildings, streets, parks, offices, etc. is considered.

The A-tables of Appendix I provide the estimated total release fractions of the production volume (emission factors) to air, (waste) water and industrial soil during production, formulation, industrial/professional use, private use, and recovery, according to their industrial category. The production volume is defined as the total tonnage of a substance brought to the European market in one year, i.e. the total volume produced in the EU plus the total amount imported into the EU, and minus the total volume exported from the EU excluding the volume of

the substance present in products imported/exported. The total volume released is averaged over the year and used for the PECregional calculation.

The B-tables of Appendix I are used for the determination of the releases from point sources for the evaluation of PEClocal. They provide the fraction of the total volume released that can be assumed to be released through a single point source, and the number of days during which the substance is released, thus allowing the daily release rate at a main point source to be calculated.

Despite the need for applying expert judgement when determining the fraction of main source, the following general guidelines for the emission estimation should be applied:

- for production the input for the regional production volume is by default set at the EU production volume, which is also used as input for the B-tables. Based on the information available to the rapporteur on the number of production sites, size distribution and geographic distribution it can be decided to apply a 10% rule, where it is assumed that 10% of the amount that is produced and used in the EU is produced/used within a region and it is subsequently assumed that the size of the main local source can be obtained by multiplying this amount with the fraction of main source from the B-tables. Alternatively it can be decided to use another percentage or to use specific values as input for the regional model (e.g. the emissions from the largest source or the emissions from the largest emitter) where this reflects a more realistic worst case. Similarly this information can be used to set the fraction of main source for the local exposure calculation. It should be noted that if site-specific data are available then it can be the case that the largest site is not the largest source of emissions;
- for formulation and processing (industrial use) a similar approach as for production is used: by default the EU volume is used as input for the region as well as for the B-tables **unless** it can be shown/is known that a large number of sites with a reasonable European distribution exists for the specific formulation/processing step of the substance involved. In that case again it can be decided to apply the 10% rule, to use another percentage or to use specific values. Whether or not the available information is sufficient for a specific substance will depend on the expert judgement by the rapporteur;
- for private use the 10% rule is applied by default both for the input of the regional volume and for the input volume for the B-table in agreement with the assumption of 10% of the use occurring in the region.

It must be realised that depending on the IC/UC combination this approach may in some cases lead to unreasonable worst-case assumptions, especially for the estimation of the emissions during formulation/processing. Hence, a case-by-case assessment using expert judgement remains warranted. For new substances the default should be overwritten anyway because it may be assumed that in most cases just one or at the most a few producers exist.

To obtain the best entry to the tables for emission factors, Appendix I also contains a list of synonyms for functions of substances. The synonyms and their definitions have been derived from the US EPA ChemUSES list (US EPA, 1980).

In general, the data supplied by industry will help to find the correct entry to the release tables apart from the classification specified in Chapter 5.

The production volume is expressed in tonnes/year in the data set and denoted by PRODVOL. TONNAGE is the volume of substance that is used for subsequent life-cycle stages. In the emission tables of Appendix IB, PRODVOL must be used for T when estimating releases at production whereas TONNAGE should be used as T for the subsequent life-cycle stages. If at the disposal

stage the substance is recovered this amount should be added to the tonnage of the relevant life-cycle stages. Note that IMPORT and EXPORT refer to the EU, not Member States within the EU.

$$TONNAGE = PRODVOL + IMPORT - EXPORT \quad (4)$$

Explanation of symbols

PRODVOL	production volume of substance	[tonnes · yr^{-1}]	data set
IMPORT	volume of substance imported	[tonnes · yr^{-1}]	data set
EXPORT	volume of substance exported	[tonnes · yr^{-1}]	data set
TONNAGE	tonnage	[tonnes · yr^{-1}]	

The release (in tonnes.yr^{-1}) per stage of the life-cycle and to every environmental compartment is calculated with the equations given in Appendix IA and denoted by $RELEASE_{i,j}$ (where i is the stage in the life-cycle and j is the compartment):

i	**stage of the life-cycle**	***j***	**compartment**
1	production	a	air
2	formulation	w	water
3	industrial/professional use	s	industrial soil (regional only)
4	private use		
5	service life		
6	waste disposal (including waste treatment and recovery)		

The following table presents the variables used as input for the emission tables in Appendix I, and the releases which are the output from emission tables and the calculation routine of Appendix I.

Input

MAINCAT	main category (for existing substances)	[-]	data set
INDCAT	industrial category	[-]	data set
USECAT	use category	[-]	data set
TONNAGE	tonnage (production volume + import - export)	[tonnes · yr^{-1}]	eq. (4)
PRODVOL	production volume of substance	[tonnes · yr^{-1}]	data set
SOL	water solubility	[mg · l^{-1}]	data set
VP	vapour pressure	[Pa]	data set
BOILPT	boiling point (for some estimations)	[°C]	data set
Specific information on the use pattern of the substance			

Output

$RELEASE_{i,j}$	release to compartment *j* during life-cycle stage *i*	[-]	App. IA
$Fmainsource_i$	fraction of release at the local main source at life-cycle stage *i*	[-]	App. IB
$Temission_i$	total number of days for the emission at life-cycle stage *i*	[d]	App. IB

For each stage other than production, the losses in the previous stage are taken into account (see calculation in Appendix I). Releases during production are not taken into account in the other stages, as generally, these releases will not have been considered in the reported production volume. In certain cases this might lead to total releases exceeding 100%. The rapporteur must

specify if releases during each stage are relevant or not. If the release during a certain life stage is not applicable, the release fraction will be set to zero.

Furthermore, few quantitative methods have been developed for estimation of the emissions during the service life of articles containing the substance (main category II) e.g. for emission of a flame retardant in plastics used for TV-sets, radios etc. However, though quantitative methodologies are at present scarce for these types of emissions, preliminary quantitative estimations may be performed on a case-by-case basis (see Section 2.3.3.5).

After accounting for losses during the six stages of the life-cycle, the part of the tonnage that remains is assumed to end up in waste streams completely. Quantitative methods for estimating emissions at the disposal stage are currently available for municipal waste incineration and municipal landfills. However, at present there is not sufficient information available, to set up an emission scenario which is representative at EU level. Nevertheless, preliminary quantitative estimations modelling a reasonable worst case for the regional scenario may be performed on a case-by-case basis. Quantitative methods for the various types of waste operations aiming at recovery are at the stage of development. Preliminary quantitative estimations may be performed on a case-by-case basis (see Sections 2.3.3.6 and 2.3.7.2).

For local emissions for every environmental compartment, the main point source and each stage of the life-cycle is considered. The emission rate is given averaged per day (24 hours). This implies that, even when an emission only takes place a few hours a day, the emission will be averaged over 24 hours. Emissions to air and water will be presented as release rates during an emission episode. Local emissions can be calculated for each stage of the life-cycle and each compartment:

$$Elocal_{i,j} = Fmainsource_i \bullet \frac{1000}{Temission_i} \bullet RELEASE_{i,j} \quad (5)$$

Explanation of symbols

$RELEASE_{i,j}$	release during life-cycle stage *i* to compartment *j*	[tonnes · yr^{-1}]	App. IA
$Fmainsource_i$	fraction of release at the local main source at life-cycle stage *i*	[-]	App. IB
$Temission_i$	number of days per year for the emission in stage *i*	[d · yr^{-1}]	App. IB
$Elocal_{i,j}$	local emission during episode to compartment *j* during stage *i*	[kg · d^{-1}]	

For local release estimates, point sources (and therefore, presumably single stages of the life-cycle) need to be identified. It will normally be necessary to assess each stage of the life-cycle to determine whether adverse effects can occur since decisions need to be made to clarify or reduce any identified risk for all life-cycle stages. This is not required if it is obvious that a certain stage is negligible.

For the regional scale assessments, the release fractions for each stage of the life-cycle need to be summed for each compartment. The emissions are assumed to be a constant and continuous flux during the year. Regional emissions can be calculated as:

$$Eregional_j = \frac{1000}{365} \bullet \sum_{i=1}^{6} RELEASE_{i,j} \quad (6)$$

Explanation of symbols

$RELEASE_{i,j}$	release during life-cycle stage *i* to compartment *j*	[tonnes · yr^{-1}]	App. IA
$Eregional_j$	total emission to compartment *j* (annual average)	[kg · d^{-1}]	

When assessing the releases on local and regional scales, the following points must be noted:

- in particular High Production Volume Chemicals (HPVCs) often have more than one application, sometimes in different industrial categories. For these substances, the assessment proceeds by breaking down the production volume for every application according to data from industry. For the local situation, in principle, all stages of the life-cycle need to be considered for each application. Where more than one stage of the life-cycle occurs at one location, the PEClocal shall be calculated by summing all the relevant emissions from that location. For releases to wastewater, only one point source for the local STP is considered. For the regional situation, the emissions to each compartment have to be summed for each stage of the life-cycle and each application. The regional environmental concentrations are used as background concentrations for the local situation;
- if substances are applied in products with an average life span of many years, after the initial arrival of the products onto the market the yearly emissions to the environment will increase. However, after a certain number of years with similar use of the products a steady-state situation will be reached. Examples are a plastic article or a paint coating where the substance assessed is applied as a plasticiser (see also Section 2.3.3.5).

Emission reduction techniques have not been taken into account in the tables of Appendix IA as the kind of techniques applied (with possibly large differences in efficiencies) as well as the degree of penetration may differ between Member States or industry sectors. Only when for a certain process a specific reduction measure is common practice this will be taken into account. In all other cases, reasonable worst-case applies.

2.3.3.4 Intermittent releases

Many substances are released to the environment from industrial sources as a result of batch, rather than continuous, processes. In extreme cases, substances may only be emitted a few times a year. Since the PECs associated with industrial releases can take into account both the amount released and the number of days of emission, the magnitude of the PECs in the risk assessment should not be affected. PEClocal is always calculated on the basis of a daily release rate, regardless of whether the discharge is intermittent or continuous. It represents the concentration expected at a certain distance from the source on a day when discharge occurs. The discharge is always assumed to be continuous over the 24-hour period. On the other hand, PECregional is calculated using the annual release rate. It represents the steady-state concentration to be expected, regardless of when the discharge occurred.

Intermittent release needs to be defined, although rapporteurs will have to justify the use of this scenario on a case-by-case basis. Intermittent release can be defined as “intermittent but only recurring infrequently i.e. less than once per month and for no more than 24 hours”.

This would correspond to a typical batch process only required for a short period of the year (releases to the environment may be only of limited duration). Thus, for the aquatic compartment, transport processes may ensure that the exposure of aquatic organisms is of short duration. Calculation of the likely exposure period should take into account the potential of a substance to substantially partition to the sediment. Such partitioning, while reducing the

calculated $PEClocal_{water}$ may also increase the exposure time by repartitioning to the water phase over an extended period. For intermittent releases to the aquatic compartment a dedicated PNEC is used in the risk characterisation (see Section 3.2.2) that has been derived using a method differing from the usual one.

Where the batch process occurs more frequently than above or is of a longer duration, protection against short-term effects cannot be guaranteed because fish, rooted plants and the majority of the macro-invertebrates are more likely to be exposed to the substance on the second and subsequent emissions. When intermittent release is identified for a substance, this is not necessarily applicable to all releases during the life-cycle.

2.3.3.5 Emissions during service-life of long-life articles

Long-life articles are here defined as articles having a service-life longer than one year. Substances in such articles may accumulate in society (landfills excluded). The emissions from long-life articles can be expected to be highest at steady state (i.e. when the flow of an article into society equals the outflow, see **Figure 5**). Estimating the emissions often requires knowledge of the substance use pattern in the preceding years.

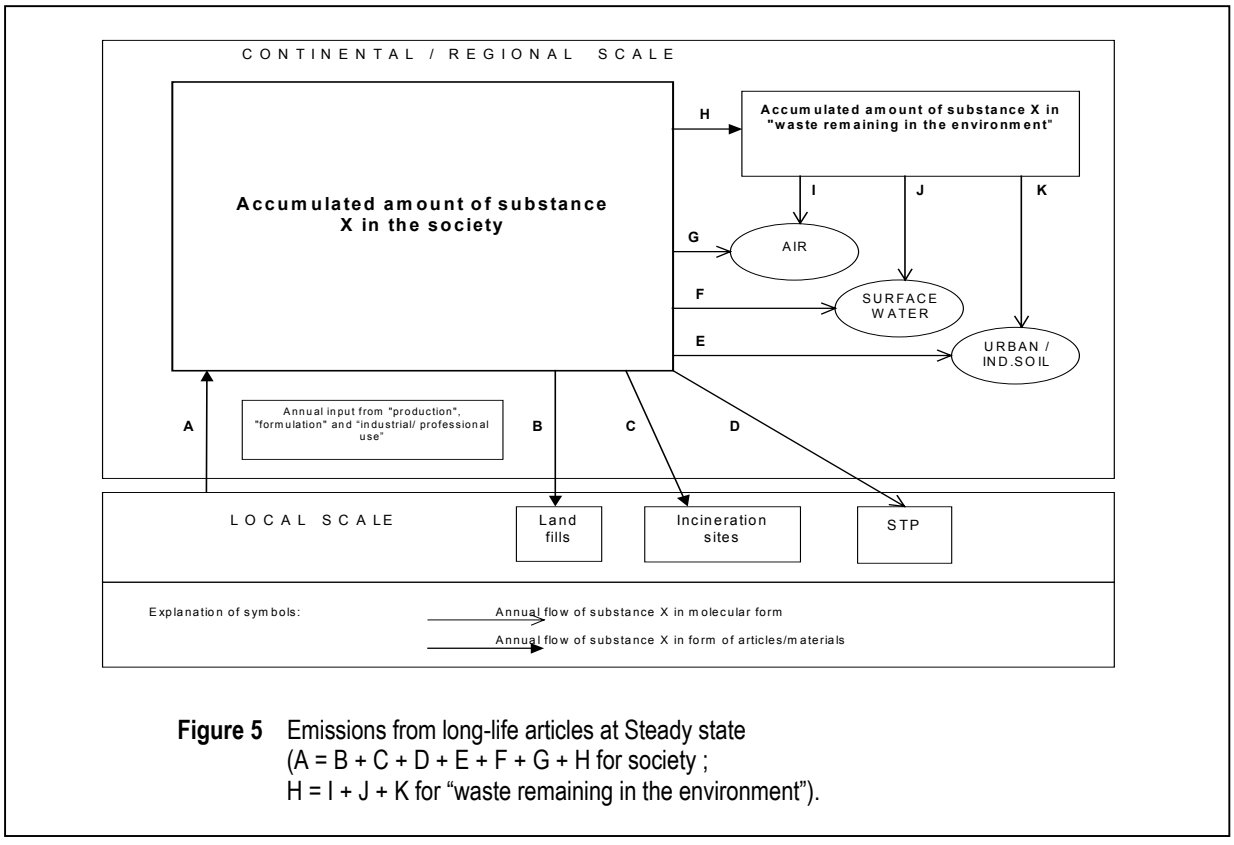

Figure 5 Emissions from long-life articles at Steady state
(A = B + C + D + E + F + G + H for society ;
H = I + J + K for "waste remaining in the environment").

There are several mechanisms for diffuse emission such as evaporation, leaching, corrosion, abrasion and weathering effects. An additional release route that in some cases is of importance is when a substance diffuses from one material into another (e.g. from glue material into construction material). Substances that are slowly emitted from long-life materials are often characterised by inherent properties such as low water solubility and low vapour pressure (e.g.

semi-volatile substances). Particulate emissions will have different fate and behaviour properties compared to molecular emissions e.g. lower bioavailability and longer persistence. However, in the absence of more detailed data concerning adsorption/bioavailability/persistence, the substance content in small particles can be handled as if it was distributed in molecular form.

The emission from articles can be assumed to be proportional to the surface area. It is, however, not always possible to estimate this area. Weight based emission factors are then used.

For the molecular emission of additives from long-life materials, the emission can normally be expected to be highest in the beginning of the use period (due to diffusion mechanisms). The opposite situation occurs for solid metal products where the particle emission can be expected to be highest at the end of the use period. It is necessary to be aware that the emission factors are normally an average for the whole service life.

There are no A-tables available for estimating emissions from the use of long-life articles. Instead the "emission scenario documents" in Chapter 7 can be used. If the use of articles is not covered by the emission scenario documents, the release estimations has to be done on a case by case basis.

The service life of an article can be defined as the average lifetime of the article. If a significant proportion of an article/material/substance is re-used or recycled leading to a second service life this should be considered in the exposure assessment. Depending on the re-use/recycle pattern this can be handled in different ways:

- if the recycling of an article leads to a second service life with the same or a similar use as the first service life this can be accounted for by adequately prolonging the first service life;
- if the recycling of an article leads to a second service life different from the first service life, emissions from both service lives are calculated separately;
- if the substance/material is recovered and used as raw material for production of new articles this amount should be added to the appropriate life-cycle stage (formulation, industrial/professional use), if not already accounted for.

The calculations of emissions from long-life articles can be performed as follows:

1) estimation of the service life of the article;
2) estimation of emission factors for the substance from the actual material (e.g. fraction/tonnes or $mg.m^{-2}$ surface area). If emission data are missing:
   - compare with similar articles described in chapter 7 (ESDs);
   - search for data in the literature;
   - use a worst-case assumption or if necessary request for an emission study;
3) calculation of the total releases of substance from articles at steady state.

Assuming constant annual input of the substance and a constant emission factor the equation for the releases to a specific compartment and for the total of all compartments can be written as:

$$RELEASEtot\_steadystate_{i,j,k} = F_{i,j} \cdot Qtot\_accum\_steadystate_k \quad (7)$$

and:

$$RELEASEtot\_steadystate_{i,total,k} = F_{i,total} \cdot Qtot\_accum\_steadystate_k \quad (8)$$

where the amount accumulated in product *k* in the society at the end of service life (steady state) can be calculated as:

$$Qtot\_accum\_steadystate_k = Qtot_k \cdot \sum_{y=1}^{Tservice_k} (1 - F_{i,total})^{y-1} \quad (9)$$

In situations where the emission factor is low (< 1%.yr^{-1}) and the service life of the product is not very long, the emissions and accumulation at steady state (eq. 7-9) can be simplified as:

$$RELEASEtot\_steadystate_{i,j,k} = F_{i,j} \cdot Qtot_k \cdot Tservice_k \quad (10)$$

$$RELEASEtot\_steadystate_{i,total,k} = F_{i,total} \cdot Qtot_k \cdot Tservice_k \quad (11)$$

$$Qtot\_accum\_steadystate_k = Qtot_k \cdot Tservice_k \quad (12)$$

Explanation of symbols

$F_{i,,j}$	Fraction of tonnage released per year (emission factor) during life-cycle stage i (service life) to compartment j	[-]	data set [1]
$F_{i,total}$	Fraction of tonnage released per year (emission factor) during life-cycle stage i (service life) to all relevant compartments	[-]	data set [2]
RELEASEtot_steady state$_{i,j,k}$	Annual total release to compartment j at steady state for product k	[tonnes · yr^{-1}]	
RELEASEtot_steady state$_{i,total,k}$	Annual total releases to all relevant compartments at steady state for product k	[tonnes · yr^{-1}]	
$Qtot_k$	Annual input of the substance in product k	[tonnes · yr^{-1}]	data set
Qtot_accum_steady state$_k$	Total quantity of the substance accumulated in product k at steady state	[tonnes]	
$Tservice_k$	Service life of product k	[yr]	data set

1) Alternatively use equation 16
2) Alternatively use equation 17

The annual total amount that will end up as waste from product *k* at the end of service life at steady state (b+c+h in **Figure 5**) can be written as (assuming no degradation within the article):

$$QWASTEtot\_steadystate_k = Qtot_k - RELEASEtot\_steadystate_{i,total,k} \quad (13)$$

Explanation of symbols

QWASTEtot_steady state$_k$	Total quantity of the substance in product k ending up as waste at steady state	[tonnes · yr^{-1}]	
$Qtot_k$	Annual input of the substance in product *k*	[tonnes · yr^{-1}]	data set
RELEASEtot_steady state$_{i,total,k}$	Annual total releases to all relevant compartments at steady state for product *k*	[tonnes · yr^{-1}]	eq. (8)

Using a 10% default the annual regional release from article k to compartment j and for the total of all compartments can be calculated as:

$$RELEASEreg\_steadystate_{i,j,k} = RELEASEtot\_steadystate_{i,j,k} \cdot 0.1 \quad (14)$$

and:

$$RELEASEreg\_steadystate_{i,total,k} = RELEASEtot\_steadystate_{i,total,k} \cdot 0.1 \quad (15)$$

Explanation of symbols

RELEASEreg_steady state$_{i,j,k}$	Annual regional release to compartment *j* at steady state for product *k*	[tonnes · yr^{-1}]	
RELEASEreg_steady state$_{i,total,k}$	Annual regional release to all relevant compartments at steady state for product *k*	[tonnes · yr^{-1}]	
RELEASEtot_steady state$_{i,j,k}$	Annual total release to compartment *j* at steady state for product *k*	[tonnes · yr^{-1}]	eq. (7/10)
RELEASEtot_steady state$_{i,total,k}$	Annual total releases to all relevant compartments at steady state for product *k*	[tonnes · yr^{-1}]	eq. (8/11)

These regional diffuse releases are then added to the regional emissions calculated from non-diffuse emissions (Eregional$_j$; eq. (6))

If an emission factor is available as release per surface area, it can be converted to a product specific "fraction of tonnage released" ($F_{i,j}$ and $F_{i,total}$):

$$F_{i,j}\ (\text{product specific}) = \frac{\text{EMISSIONarea}_{i,j,k} * 1000}{\text{THICK}_k * \text{CONC}_k} \quad (16)$$

and:

$$F_{i,total}\ (\text{product specific}) = \frac{\text{EMISSIONarea}_{i,total,k} * 1000}{\text{THICK}_k * \text{CONC}_k} \quad (17)$$

Explanation of symbols

$F_{i,j}$	Fraction of tonnage released per year (emission factor) during life cycle stage *i* (service life) to comparment *j* from product *k*	[yr^{-1}]	
$F_{i,total}$	Fraction of tonnage released per year (emission factor) during life cycle stage *i* (service life) to all relevant compartments from product *k*	[yr^{-1}]	
CONC$_k$	Concentration of substance in product *k*	[kg · dm^{-3}]	data set
EMISSIONarea$_{i,j,k}$	Annual amount of substance emitted per area from product *k* to compartment *j*	[g · m^{-2} · yr^{-1}]	data set
EMISSIONarea$_{i,total,k}$	Annual total of amount substance emitted per area from product *k*	[g · m^{-2} · yr^{-1}]	data set
THICK$_k$	Thickness of the emitting material in product *k*	[mm]	data set

If the area based emissions can be expected to decrease with decreasing concentration in the product the equations 7-8 above are used. If the emission is expected to be independent of the

remaining amount of the substance in the product, e.g. corroding metals, the simplified equations 10-11 are used.

If the amount of a substance in use in the society has not reached steady state and the accumulation is still ongoing, the calculated PEC will represent a future situation. If this is the case this should be considered when comparing PEC with monitoring data.

Releases from articles will normally only contribute to the continental and regional releases. The emissions from indoor uses can be released to wastewater and therefore be regarded as a point source (stream "d" in **Figure 5**). Also outdoor uses may cause releases to STP if the storm water system is connected to the STP. This has to be considered case by case. For the calculation of a local scenario the B-table in Appendix I for Industry Category 5 Personal/domestic shall be used.

Quantitative methods for estimating emissions from waste remaining in the environment are currently not available. Therefore such releases have to be considered on a case-by-case basis. As for substances in long-life articles, substances in "waste remaining in the environment" will also accumulate. As a simplification the emissions at steady state can be assumed to be equal to the annually formed amount of "waste remaining in the environment" (see **Figure 5**). If the degradation rate of the substance in the waste material is known, this should be taken into consideration. When the emission of a substance from waste remaining in the environment is very slow it will take a long time to reach steady state. In that case the calculated emission may reflect a future situation.

As for emissions from articles releases from waste remaining in the environment will also contribute mainly to the continental and regional releases.

2.3.3.6 Emissions from waste disposal

If the major share of a substance placed on the market remains in chemical products or articles at the end of their service life (releases during production, processing and use are comparatively small), the waste life-cycle stage of the substance may need particular attention. This refers e.g. to organic substances in landfills and metals in waste incineration processes. The underlying criterion for considering waste emissions in the risk assessment of substances, is that the waste stage will contribute significantly to the overall human exposure or environmental concentration in comparison to the emissions from other parts of the life-cycle of the substance (e.g. production and use stages). If this is not the case, waste considerations could be excluded from the assessment process and general risk management measures based on EU waste legislation should be sufficient.

For certain types of substances, e.g. metals and persistent and toxic substances releases from waste may be slow compared to the release from the production and use phase but nevertheless the continued long-term release after use could be of concern. On a case-by-case basis, these aspects may be addressed in the risk assessment.

To guide the decision whether an estimation of the releases from the waste stage is pertinent, the following considerations may be used.

First, on the basis of the production volume and the use pattern a preliminary assessment on the volume that may end up in the waste streams should be performed. In doing so the toxicity and other adverse effects of the substance and of possible breakdown products should be taken into

account to qualify the significance of the possible impact of such a volume entering the waste stream. Even a small volume of a highly toxic compound may be of concern.

Subsequently, information on anaerobic degradation in landfills or conditions simulating conditions in landfills may indicate that further assessment may not be needed. Water solubility, adsorption/desorption in soil (under landfill conditions) or if available from leaching experiments could also be included in the evaluation as an indicator for leaching potential. However, it is noted that even sorbed substances may leave the landfill via particle transport with leachates.

The substance may also leave the landfill with the produced landfill gas. The Kow and Henry's Law constant as well as the tropospheric persistency may be used to indicate whether the release through landfill gas may be of significance. A proposal for possible trigger values can be found in Danish EPA (2001).

For incineration, inorganic substances are the predominant substances of concern. The concern is especially associated with possible leaching of such substances from incineration products whether landfilled or used e.g. for road construction. Furthermore, substances that contain halogens need special attention due to the possible formation of hazardous substances during incineration.

In order to evaluate whether emissions from incineration of a substance containing an inorganic substance of concern should be included in the risk assessment, the predicted occurrence of the substance in a waste stream should be compared with typical background-ranges. If a substance or a specific use of a substance may contribute unduly to the influent concentration further release calculation should be carried out.

2.3.3.7 Delayed releases from waste disposal and dilution in time

Releases from the waste life stage may occur several decades after production and processing of the substance under assessment. These delays are determined, inter alia, by:

- the service life span of the substance as such, or in a chemical product or article;
- intermediate storage after service life before waste collection (e.g. exhausted batteries);
- exposure of residues from waste incineration to water. This source could be of particular relevance if the residues are re-introduced into the market as products (e.g. building material) exposed to water;
- intensity of gas production in landfills;
- exposure of landfilled waste to water and deterioration of the landfill bottom liner.

The releases from landfills and residues from waste incineration residues usually take place over a long time period. Hence the daily or annual release may result in a very small PEC. If available, monitoring data may be a valuable source of information (see Section 2.2.1). The need for a long-term release assessment should be decided on a case-by-case basis, in particular for metals or organic substances that are persistent and toxic.

2.3.4 Characterisation of the environmental compartments

In this section, the following parameters are derived:

- definition of the standard environmental characteristics (**Table 5**);

- bulk densities for soil, sediment, and suspended matter.

For the derivation of PECs at the local and regional scale, one standardised generic environment needs to be defined since the general aim is to obtain conclusions regarding risks of the substance at EU level. The characteristics of the real environment will, obviously, vary in time and space. In **Table 5**, average or typical default values are given for the parameters characterising the environmental compartments (the values are chosen equal on both spatial scales). The standard assessment needs to be performed with the defaults, as given in **Table 5**. When more specific information is available on the location of the emission sources, this information can be applied in refinement of the PEC by deviating from the parameters of **Table 5**.

Several other generic environmental characteristics, mainly relevant for the derivation of PECregional (e.g. the sizes of the environmental compartments, mass transfer coefficients) are given in Section 2.3.8.7 (**Tables 12-14**).

Table 5 Definition of the standard environmental characteristics

Parameter	Symbol	Unit	Value
General			
Density of the solid phase	RHOsolid	$[kg_{solid} \cdot m_{solid}^{-3}]$	2,500
Density of the water phase	RHOwater	$[kg_{water} \cdot m_{water}^{-3}]$	1000
Density of air	RHOair	$[kg_{air} \cdot m_{air}^{-3}]$	1.3
Temperature (12°C)	TEMP	[K]	285
Surface water			
Concentration of suspended matter (dry weight)	$SUSP_{water}$	$[mg_{solid} \cdot l_{water}^{-1}]$	15
Suspended matter			
Volume fraction solids in susp. matter	$Fsolid_{susp}$	$[m_{solid}^3 \cdot m_{susp}^{-3}]$	0.1
Volume fraction water in susp. matter	$Fwater_{susp}$	$[m_{water}^3 \cdot m_{susp}^{-3}]$	0.9
Weight fraction organic carbon in susp. solids	Foc_{susp}	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.1
Sediment			
Volume fraction solids in sediment	$Fsolid_{sed}$	$[m_{solid}^3 \cdot m_{sed}^{-3}]$	0.2
Volume fraction water in sediment	$Fwater_{sed}$	$[m_{water}^3 \cdot m_{sed}^{-3}]$	0.8
Weight fraction organic carbon sediment solids	Foc_{sed}	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.05
Soil			
Volume fraction solids in soil	$Fsolid_{soil}$	$[m_{solid}^3 \cdot m_{soil}^{-3}]$	0.6
Volume fraction water in soil	$Fwater_{soil}$	$[m_{water}^3 \cdot m_{soil}^{-3}]$	0.2
Volume fraction air in soil	$Fair_{soil}$	$[m_{air}^3 \cdot m_{soil}^{-3}]$	0.2
Weight fraction organic carbon in soil solids	Foc_{soil}	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.02
Weight fraction organic matter in soil solids	Fom_{soil}	$[kg_{om} \cdot kg_{solid}^{-1}]$	0.034

Each of the compartments soil, sediment, and suspended matter is described as consisting of three phases: air (only relevant in soil), solids, and water. The bulk density of each compartment is thus defined by the fraction and bulk density of each phase. Both the fractions solids and water, and the total bulk density are used in subsequent calculations. This implies that the bulk

density of a compartment cannot be changed independently of the fractions of the separate phases and vice versa.

The bulk densities of the compartments soil, sediment, and suspended matter are defined by the fractions of the separate phases:

$$RHO_{comp} = Fsolid_{comp} \bullet RHOsolid + Fwater_{comp} \bullet RHOwater + Fair_{comp} \bullet RHOair \quad with\ comp \in \{soil, sed, susp\} \tag{18}$$

Explanation of symbols

Fx_{comp}	fraction of phase x in compartment comp	[$m^3 \cdot m^{-3}$]	Table 5
RHO*x*	density of phase *x*	[$kg \cdot m^{-3}$]	Table 5
RHO_{comp}	wet bulk density of compartment comp	[$kg \cdot m^{-3}$]	

Application of the formulas above for the values mentioned leads to the following bulk densities of each standard environmental compartment:

Total bulk density of the environmental compartments

RHO_{susp}	Bulk density of (wet) suspended matter	[$kg \cdot m^{-3}$]	1,150
RHO_{sed}	Bulk density of (wet) sediment	[$kg \cdot m^{-3}$]	1,300
RHO_{soil}	Bulk density of (wet) soil	[$kg \cdot m^{-3}$]	1,700

2.3.5 Partition coefficients

In this section, the following processes are described:

- fraction of substance in air associated with aerosol;
- partitioning between air and water;
- partitioning between solids and water in soil, sediment and suspended matter.

Transport and transformation ("fate") describe the distribution of a substance in the environment, or in organisms, and its changes with time (in concentration, chemical form, etc.). Since measured data on fate processes for different compartments are usually not available, they must be extrapolated from the primary data listed in Section 2.3.2. This section describes the derivation of the partitioning processes between air-aerosol, air-water, and solids-water in the various compartments.

It should be noted that for ionising substances, partitioning behaviour between air-water and solids-water is dependent on the pH of the environment. Appendix XI gives more specific guidance for the assessment of these compounds.

Fate estimates based on "partitioning" are limited to distribution of a substance in molecular form. For substances that also will be distributed in the environment as particles (caused by abrasion/weathering of anthropogenic materials) extrapolation based on partitioning may not be relevant. In such a case the partitioning method may underestimate exposure of soil and sediment environments and overestimate the exposure of water. If the particle size is small also air distribution may occur, at least in the local perspective. There are no estimation methods available for particle distribution so this has to be dealt with on a case-by-case basis.

2.3.5.1 Adsorption to aerosol particles

The fraction of the substance associated with aerosol particles can be estimated on the basis of the substance's vapour pressure, according to Junge (1977). In this equation, the sub-cooled liquid vapour pressure should be used.

$$Fass_{aer} = \frac{CONjunge \bullet SURF_{aer}}{VP + CONjunge \bullet SURF_{aer}} \quad (19)$$

Explanation of symbols

CONjunge	constant of Junge equation	[Pa · m]	*
$SURF_{aer}$	surface area of aerosol particles	[$m^2 \cdot m^{-3}$]	*
VP	vapour pressure	[Pa]	data set
$Fass_{aer}$	fraction of the substance associated with aerosol particles	[-]	

* as a default the product of CONjunge and $SURF_{aer}$ is set to 10^{-4} Pa (Van de Meent, 1993; Heijna-Merkus and Hof, 1993).

Alternatively the octanol-air partition coefficient could be used as described by Finizio et al. (1997).

For solids, a correction of the vapour pressure is required to derive the sub-cooled liquid vapour pressure (Mackay, 1991):

$$VPL = \frac{VP}{e^{6.79 \bullet (1-\frac{TEMP_{melt}}{TEMP})}} \quad (20)$$

Explanation of symbols

TEMP	environmental temperature	[K]	285
$TEMP_{melt}$	melting point of substance	[K]	data set
VPL	sub-cooled liquid vapour pressure	[Pa]	
VP	vapour pressure	[Pa]	data set

2.3.5.2 Volatilisation

The transfer of a substance from the aqueous phase to the gas phase (e.g. stripping in the aeration tank of a STP, volatilisation from surface water) is estimated by means of its Henry's Law constant. If the value is not available in the input data set, the required Henry's Law constant and the Kair-water (also known as the “dimensionless” Henry's Law constant) can be estimated from the ratio of the vapour pressure to the water solubility. For water miscible compounds direct measurement of the Henry’s Law constant is recommended.

$$HENRY = \frac{VP \bullet MOLW}{SOL} \quad (21)$$

$$K_{air\text{-}water} = \frac{HENRY}{R \bullet TEMP} \quad (22)$$

Explanation of symbols

VP	vapour pressure	[Pa]	data set
MOLW	molecular weight	[g · mol^{-1}]	data set
SOL	solubility	[mg · l^{-1}]	data set
R	gas constant	[Pa · m^3 · mol^{-1} · k^{-1}]	8.314
TEMP	temperature at the air-water interface	[K]	285
HENRY	Henry's law constant	[Pa · m^3 · mol^{-1}]	
$K_{air\text{-}water}$	air-water partitioning coefficient	[-]	

If no reliable data for vapour pressure and/or solubility can be obtained with the present OECD guidelines, QSARs are available, but not addressed in Chapter 4 (Part III). The structural contribution method (Meylan and Howard, 1991; Hine and Mookerjee, 1975) or other (Q)SAR methods (OECD, 1993a) may be used.

2.3.5.3 Adsorption/desorption

In addition to volatilisation, adsorption to solid surfaces is the main partitioning process that drives distribution in soil, surface waters, and sediments. The adsorption of a substance to soil, sediment, suspended matter and sludge can be obtained or estimated from:

- direct measurement;
- simulation testing;
- Koc measured by adsorption studies (EC C18; OECD 106, 2000a);
- Koc measured by the HPLC-method (EC C19; OECD 121, 2001a);
- adsorption control within an inherent biodegradability test;
- if no Koc is available, it may be estimated from Kow (QSARs are given in Chapter 4).

It should be noted that for surfactants the octanol/water partition coefficient (Kow) is experimentally difficult to determine and this parameter may not be sufficiently descriptive of surface activity or adsorption/desorption (surfactant behaviour).

If no measured data are available for a specific adsorbing material, it is assumed that all adsorption can be related to the organic matter of the medium, viz. standardisation to Koc (this is only valid for non-ionic substances) based on the organic carbon content of different media (e.g. soil, sediment, suspended matter, sewage sludge). For organic, non-ionic substances, Koc can be estimated from Kow as outlined in Chapter 4. The equation for "nonhydrophobic" substances is preferred as default. For specific groups of substances, other QSARs are given in chapter 4. For ionic substances, a measured adsorption coefficient is needed, or it may be possible to first investigate how significant the value might be by using a high value of Koc in the assessment. Cationic substances are generally known to adsorb strongly.

For water soluble, highly adsorptive substances the use of Kow as input into SimpleTreat may lead to an overestimation of the aquatic exposure concentration. SimpleTreat will predict a low elimination on the basis of the log Kow (and small Henry's Law constant), while adsorption onto sludge may be a significant elimination mechanism for these substances.

In the absence of better adsorption/desorption data, the Zahn-Wellens elimination level can be used as an estimate of the extent of adsorption to sludge. The 3h value is recommended. For slowly adsorbing substances, consideration could be given to the hydraulic retention time in a STP (default is 6.8 h). Values beyond 24 h would not normally be used. Where data are not available for adsorption up to 24 hours, data from time scales beyond this can only be used if adsorption is the only removal mechanism, with an upper limit of 7 d.

The solid-water partition coefficient (Kp) in each compartment (soil, sediment, suspended matter) can be calculated from the Koc value, and the fraction of organic carbon in the compartment. Initially, the fraction of organic carbon in the standard environment should be used, as given in **Table 5**.

$$Kp_{comp} = Foc_{comp} \bullet Koc \quad with\ comp \in \{soil,\ sed,\ susp\} \tag{23}$$

Explanation of symbols

Koc	partition coefficient organic carbon-water	[l · kg^{-1}]	data set/Ch. 4
Foc_{comp}	weight fraction of organic carbon in compartment *comp*	[kg · kg^{-1}]	Table 5
Kp_{susp}	partition coefficient solid-water in suspended matter	[l · kg^{-1}]	
Kp_{sed}	partition coefficient solid-water in sediment	[l · kg^{-1}]	
Kp_{soil}	partition coefficient solid-water in soil	[l · kg^{-1}]	

Kp is expressed as the concentration of the substance sorbed to solids (in $mg_{chem} \cdot kg_{solid}^{-1}$) divided by the concentration dissolved in porewater ($mg_{chem} \cdot l_{water}^{-1}$). The dimensionless form of Kp, or the total compartment-water partitioning coefficient in $(mg \cdot m_{comp}^{-3})/(mg \cdot m_{water}^{-3})$, can be derived from the definition of the soil in three phases:

$$K_{comp\text{-}water} = \frac{Ctotal_{comp}}{Cporew_{comp}}$$

$$K_{comp\text{-}water} = Fair_{comp} \bullet K_{air\text{-}water} + Fwater_{comp} + Fsolid_{comp} \bullet \frac{Kp_{comp}}{1000} \bullet RHOsolid \tag{24}$$

$$with\ comp \in \{soil,\ susp,\ sed\}$$

Explanation of symbols

$Fwater_{comp}$	fraction water in compartment *comp*	[m^3 · m^{-3}]	Table 5
$Fsolid_{comp}$	fraction solids in compartment *comp*	[m^3 · m^{-3}]	Table 5
$Fair_{comp}$	fraction air in compartment comp (only relevant for soil)	[m^3 · m^{-3}]	Table 5
RHOsolid	density of the solid phase	[kg · m^{-3}]	2,500
Kp_{comp}	solids-water part. coeff. in compartment *comp*	[l · kg^{-1}]	eq. (23)
$K_{air\text{-}water}$	air-water partitioning coefficient	[-]	eq. (22)
$K_{soil\text{-}water}$	soil-water partitioning coefficient	[m^3 · m^{-3}]	
$K_{susp\text{-}water}$	suspended matter-water partitioning coefficient	[m^3 · m^{-3}]	
$K_{sed\text{-}water}$	sediment-water partitioning coefficient	[m^3 · m^{-3}]	

2.3.6 Abiotic and biotic degradation rates

In this section, the following processes are described:

- hydrolysis in surface water;
- photolysis in surface water and in the atmosphere;
- biodegradation in the sewage treatment plant;
- biodegradation in the environmental compartments (surface water, soil, sediment).

Transport and transformation ("fate") describe the distribution of a substance in the environment, or in organisms, and its changes with time (in concentration, chemical form, etc.), thus including both biotic and abiotic transformation processes. In general, the assessment of degradation processes should be based on data, which reflect the environmental conditions as realistically as possible. Data from studies where degradation rates are measured under conditions that simulate the conditions in various environmental compartments are preferred. The applicability of such data should, however, be judged in the light of any other degradation data including results from screening tests. Most emphasis is put on the simulation test results but in the absence of simulation test data, degradation rates and half-lives have to be estimated from screening test data.

For substances where a range of degradation data is available, a "weight of evidence" approach should be employed. When more than one simulation test result is available, a suitable half-life in the higher end of the observed range should be selected taking into account the realism, relevance, quality and documentation of the studies in relation to environmental conditions. When more than one screening test result is available, positive test results should be considered valid, irrespective of negative results, when the scientific quality is good and the test conditions are well documented, i.e. guideline criteria are fulfilled, including the use of non-adapted inoculum (cf. OECD, 2001c). The results of screening tests may be negative due to toxic effects of the test substance, whereas simulation tests employing a low concentration of the test substance may give a more realistic estimate of the degradation in the environment. By using all available degradability test data in this way, it is possible to establish a comprehensive evaluation of the degradability of the substance.

In this section, methods for derivation of degradation rate constants are described for abiotic degradation (hydrolysis and photolysis) and biotic degradation (in soil, sediment, water, and sewage treatment). For hydrolysis and photolysis, only primary degradation is measured. In general, risk assessment focuses on the parent compound. Nevertheless, if stable degradation products are formed, the risk assessment should include these. It is possible that the rate of reaction is such that only the products need to be considered, or in intermediate cases both the substance and the degradation products will require consideration. It is important to have information about which chemical species were responsible for any effects that were observed in the aquatic toxicity studies.

Where substances degrade by complex interaction mechanisms, for example abiotic degradation followed by biodegradation, and where there are no internationally recognised protocols for simulation tests, the use of relevant field data could be considered provided that the kinetics of full mineralisation or formation of possible metabolites have been determined.

2.3.6.1 Hydrolysis

Values for the half-life (DT50) of a hydrolysable substance can be converted to degradation rate constants, which may be used in the models for calculating PEClocal and especially PECregional. The results of a ready biodegradability study will show whether or not the hydrolysis products are themselves biodegradable. Similarly, for substances where DT50 is less than 12 hours, environmental effects are likely to be attributed to the hydrolysis products rather than to the parent substance itself. These effects should also be assessed. QSAR methods are available for certain groups of substances, e.g. the EPIWIN program (US EPA, 2002) and other methods described in Chapter 4.

For many substances, the rate of hydrolysis will be heavily dependent on the specific environmental pH and temperature and in the case of soil, also moisture content. For risk assessment purposes for fresh water, sediment and soil, a pH of 7 and a temperature of 12°C (285 K) will normally be established which conform to the standard environmental parameters of **Table 5**. However, for some substances, it may be necessary to assume a different pH and temperature to fully reflect the potential of the substance to cause adverse effects. This may be of particular importance where the hydrolysis profile shows significantly different rates of hydrolysis over the range pH 4 - 9 and the relevant toxicity is known to be specifically caused by either the stable parent substance or a hydrolysis product.

Rates of hydrolysis always increase with increasing temperature. When hydrolysis half-lives have been determined in standard tests, they should be recalculated to reflect an average EU outdoor temperature by the equation:

$$DT50(X°C) = DT50(t) \cdot e^{(0.08 \cdot (T-X))} \tag{25}$$

where X = 12°C for fresh water. When it is documented for a specific substance that the typical pH of the environmental compartment to be assessed also affects the hydrolysis rate in addition to temperature, the most relevant hydrolysis rate should be taken or extrapolated from the results of the standard test in different pH values. Thereafter the temperature correction is to be applied, where relevant.

When the use of an alternative pH will affect the environmental distribution and toxicity by changing the nature of the soluble species, for example with ionisable substances, care should be taken to ensure that this is fully taken into account when making a final PEC/PNEC comparison.

The half-life for hydrolysis (if known) can be converted to a pseudo first-order rate constant:

$$khydr_{water} = \frac{\ln 2}{DT50\,hydr_{water}} \tag{26}$$

Explanation of symbols

$DT50hydr_{water}$	half-lifetime for hydrolysis in surface water	[d]	data set
$khydr_{water}$	first order rate constant for hydrolysis in surface water	[d^{-1}]	

2.3.6.2 Photolysis in water

In the vast majority of surface water bodies dissolved organic matter is responsible for intensive light attenuation. Thus photolysis processes are normally restricted to the upper zones of water bodies. Indirect processes like photo-sensitisation or reaction with oxygen transients ($^1O_2$, OH-radicals, ROO-radicals) may significantly contribute to the overall breakdown rate. Photochemical degradation processes in water may only become an important fate process for substances, which are persistent to other degradation processes (e.g. biodegradation and hydrolysis). The experimental determination of the quantum yield (OECD, 1992c) and the UV-absorption spectrum of the substance are prerequisites for estimating the rate of photodegradation in surface water. Due to high seasonal variation in light flux, photochemical degradation should only be based on average EU conditions. Methods to derive average degradation rates which can be used in the model calculation of PECregional are described in Zepp and Cline (1977) and Frank and Klöppfer (1989).

The following aspects have to be considered when estimating the photochemical transformation in natural water bodies:

- the intensity of the incident light depends on seasonal and geographic conditions and varies within wide ranges. For long-term considerations average values can be used while for short-term exposure an unfavourable solar irradiance (winter season) should be chosen;
- in most natural water bodies, the rate of photoreaction is affected by dissolved and suspended matter. Since the concentration of the substance under consideration is normally low compared to the concentration of e.g. dissolved humic acids, the natural constituents absorb by far the larger portion of the sunlight penetrating the water bodies.

Using the standard parameters of the regional model (i.e. a water depth of 3 m and a concentration of suspended matter of 15 mg/l), the reduction in light intensity is higher than 98% through the water column.

Indirect (sensitised) photochemical reactions should only be included in the overall breakdown rate of water bodies if there is clear evidence that this pathway is not of minor importance compared to other processes and its effectiveness can be quantified. For facilitating the complex calculation of phototransformation processes in natural waters computer programmes have been developed (e.g. ABIWAS by Frank and Klöppfer, 1989; GC-SOLAR by Zepp and Cline, 1977).

In practice it will not be possible to easily demonstrate that photodegradation in water is significant in the environment.

A value for the half-life for photolysis in water (if known) can be converted to a pseudo first-order rate constant:

$$kphoto_{water} = \frac{\ln 2}{DT50\ photo_{water}} \qquad (27)$$

Explanation of symbols

$DT50photo_{water}$	half-lifetime for photolysis in surface water	[d]	data set
$kphoto_{water}$	first order rate constant for photolysis in surface water	[d^{-1}]	

2.3.6.3 Photochemical reactions in the atmosphere

Although for some substances direct photolysis may be an important breakdown process, the most effective elimination process in the troposphere for most substances results from reactions with photochemically generated species like OH radicals, ozone and nitrate radicals. The specific first order degradation rate constant of a substance with OH-radicals (k_{OH} in $cm^3 \cdot molecule^{-1} \cdot s^{-1}$) can either be determined experimentally (OECD, 1992c) or estimated by (Q)SAR-methods and other methods described in Chapter 4 (US EPA, 2002). By relating k_{OH} to the average OH-radical concentration in the atmosphere, the pseudo-first order rate constant in air is determined:

$$kdeg_{air} = k_{OH} \bullet OHCONC_{air} \bullet 24 \bullet 3600 \quad (28)$$

Explanation of symbols

k_{OH}	specific degradation rate constant with OH-radicals	$[cm^3 \cdot molec^{-1} \cdot s^{-1}]$	data set/Ch.4
$OHCONC_{air}$	concentration of OH-radicals in atmosphere	$[molec \cdot cm^{-3}]$	$5 \cdot 10^5$ *
$kdeg_{air}$	pseudo first order rate constant for degradation in air	$[d^{-1}]$	

*The global annual average OH-radical concentration can be assumed to be 5.10^5 molecules.cm^{-3} (BUA, 1992).

Degradation in the atmosphere is an important process and it is essential to consider whether it can affect the outcome, particularly for high tonnage substances when the regional concentration may be significant. Photodegradation data in the atmosphere must be evaluated with some care. Highly persistent substances may be reported as rapidly degraded in air under environmental conditions where the chemical could be in large amounts in the gas phase. In the real environment, most of the substance may be associated to particles or aerosol and the real atmospheric half-life could be orders of magnitude higher.

2.3.6.4 Biodegradation in a sewage treatment plant

The assessment of biodegradability and/or removal in sewage treatment plants should preferably be based on results from tests simulating the conditions in treatment plants. Such a test may be the OECD 303 test (2001b) or equivalent. For further guidance on use of STP simulation test results, see Section 2.3.7.

The ready biodegradability tests that are used at the moment are aimed at measuring the ultimate biodegradability of a substance. They do not give a quantitative estimate of the removal percentage in a wastewater treatment plant. Therefore, in order to make use of the biodegradation test results that are available and requested in the present chemical legislation, it is necessary to assign rate constants to the results of the standard tests for use in STP-models. These constants are based on a relatively limited number of empirical data. However, since direct measurements of degradation rates at environmentally relevant concentrations are often not available, a pragmatic solution to this problem has been found. For the purpose of modelling a sewage treatment plant (STP), the rate constants of **Table 6** were derived from the biodegradation screening tests. All constants in **Table 6** have the following prerequisites:

- they are only used for the water-dissolved fraction of the substance. Partitioning between water and sludge phases should be calculated prior to the application of the rate constant;
- sufficiently valid data from internationally standardised tests are preferred;

Data from non-standardised tests and/or tests not performed according to the principles of GLP may be used if expert judgement has confirmed them to be equivalent to results from the standardised degradation tests on which the calculation models, e.g. SimpleTreat, are based. The same applies to STP-measured data, i.e., in-situ influent/effluent measurements.

Table 6 Elimination in sewage treatment plants: Extrapolation from test results to rate constants in STP model (SimpleTreat)

Test result	Rate constant k · (h^{-1})
Readily biodegradable [a)]	1
Readily, but failing 10-d window [a)]	0.3
Inherently biodegradable, fulfilling specific criteria [b)]	0.1
Inherently biodegradable, not fulfilling specific criteria [b)]	0
Not biodegradable	0

Notes to Table 6:

a) Ready biodegradability testing (28 d) (92/69/ EU Annex V C.4 A-F, or respectively, OECD 301A-F (1992f) or equivalent according to expert judgement).
Ready biodegradability tests are screening tests for identifying substances that, based on general experience, are assumed to undergo rapid and ultimate biodegradation in the aerobic environment. However, a negative result does not necessarily mean that the substance will not be biodegraded in, e.g., a sewage treatment plant.
The degree of ultimate degradation may be followed by determination of the loss of dissolved organic carbon (DOC), the evolution of carbon dioxide or the amount of oxygen consumed. It is generally accepted that a substance is considered to be readily biodegradable if the substance fulfils the pass criteria of a test for ready biodegradability (cf. the Annex V methods or the OECD guidelines) which may include the concept of the 10 days time window as a simple kinetic criterion. All percentage biodegradation results refer to true biodegradation i.e. mineralisation excluding abiotic elimination processes (e.g. volatilisation, adsorption). This means that corresponding data in adequate control vessels must be generated during biodegradation testing. The test may be continued beyond 28 days if biodegradation has started but does not reach the required pass criteria for final mineralisation: in this case however, the substance would not be regarded as being readily biodegradable. If the substance reaches the biodegradation pass levels within 28 days but not within the 10-day time window, a biodegradation rate constant of 0.3 h^{-1} is assumed. In case that only old ready biodegradation test results (i.e. tests executed prior to the introduction of the 10 days time window criterion and documenting only on the pass level) are available a rate constant of 0.3 h^{-1} should be applied in case the pass level is reached. Based on weight of evidence (e.g. several old test results) a rate constant of 1 h^{-1} may be justified by expert judgement.
If the substance is found to be not readily biodegradable, it is necessary to check whether it was inhibitory to microbial activity at the concentration used in the biodegradability test. If the substance is inhibitory, it may be re-tested at low, non-inhibitory concentrations in a test simulating the conditions in a sewage treatment plant (e.g. OECD guideline 303, 2001b; ISO 11733 or equivalent). If appropriate, re-testing in another more suitable ready biodegradability test (e.g. Closed Bottle test) may be considered. Re-testing in a modified ready biodegradability test at a much lower concentration (i.e. more than 10 times lower than prescribed) cannot generally be recommended because suitable simulation test methods are available.

b) Inherent biodegradability testing (28d) (87/302/EEC, respectively, OECD 302B-C (1981d-1992g) or equivalent according to expert judgement).
Inherent biodegradability tests are designed to assess whether the substance has any potential for biodegradation. A negative result will normally mean that non-biodegradability (persistence) should be assumed. A positive result, on the other hand, indicates that the substance will not persist indefinitely in the environment. In those cases where a more accurate prediction of degradation kinetics in treatment plants is required, sewage treatment plant simulation tests (e.g. OECD guideline 303, 2001b; ISO 11733 or equivalent) should be conducted.
In tests for inherent biodegradability, the test conditions are designed to be more favourable to the microorganisms in that the ratio of substance to cells is lower than in the ready tests and there is no requirement for the (bio)degradation to follow a time pattern as in the ready tests. Also, pre-exposure of the inoculum resulting in pre-adaptation of the microorganisms may be allowed. The time permitted for the study is limited to 28 days, but it may be continued for much longer; 6 months has been suggested as the maximum duration for the test. The results obtained in a test of more than 28 days are not comparable with those obtained in less than this period.
Usually, more than 70% (bio)degradation within 28 days indicates that the substance is inherently biodegradable. However, extrapolation of the results of the inherent tests should be done with great caution because of the strongly favourable conditions for biodegradation that are present in these tests. Therefore, a substance that passes an inherent test should in principle be given a rate

constant of zero. However, if it can be shown that:

- The elimination in the test can really be ascribed to biodegradation, and;
- No recalcitrant metabolites are formed, and;
- The adaptation time in the test is limited;

then a rate constant of 0.1 h^{-1} in the STP-model can be used. These qualitative criteria are transformed into the following more specific criteria that the different inherent biodegradation tests must fulfil:

Zahn-Wellens test: Pass level must be reached within 7 days, log-phase should be no longer than 3 days, percentage removal in the test before biodegradation occurs should be below 15 %.

MITI-II test: Pass level must be reached within 14 days, log-phase should be no longer than 3 days.

No specific criteria have been developed for positive results in a SCAS test. A rate constant of 0 h^{-1} will be assigned to a substance, irrespective whether it passes this test or not.

2.3.6.5 Biodegradation in surface water, sediment and soil

The rate of biodegradation in surface water, soil and sediment is related to the structure of substances, microbial numbers, organic carbon content, and temperature. These properties vary spatially and an accurate estimate of the rate of biodegradation is very difficult even if laboratory or field data are available. Fate and exposure models normally assume the following simplifications:

- the kinetics of biodegradation are pseudo-first order;
- only the dissolved portion of the substance is available for biodegradation.

Normally, specific information on biodegradability in sediment or soil is not available. Hence, rate constants for these compartments have to be estimated from the results of standardised tests.

In deeper sediment layers anaerobic conditions normally prevail. A prediction of anaerobic biodegradation from aerobic biodegradability is not possible. For testing of anaerobic biodegradation the ISO 11734 guideline is available (ISO 1995). This screening test method is designed to investigate the potential for anaerobic degradation in STP digesters.

The assessment of biodegradation in surface waters, sediments and soil should, whenever possible, be based on results from tests simulating the conditions in the relevant environmental compartments.

Temperature influences the activity of microorganisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives have been determined in simulation tests, it should be considered to recalculate the degradation rates obtained to reflect an average EU outdoor temperature by equation (25). When it is documented for a specific substance that a difference between the temperature employed in the test and the average outdoor temperature has no influence on the degradation half-life, no correction is needed.

Preference of simulation tests also applies to estimation of degradation half-life in surface waters. The draft ISO/DIS 14952-1 standard on biodegradation of organic substances at low concentration in surface waters was agreed in 1999. The ISO method has been the basis for a proposal for a new OECD guideline “Simulation test – Aerobic mineralisation in surface water” (OECD, 2001d). It is foreseen that in future results from such tests may sometimes be available or required for risk assessment of high priority substances. An assessment of the applicability of such test results should always be conducted taking into account the prescribed standard conditions for surface waters applied in the risk assessment scenarios according to this TGD relative to the conditions employed in simulation tests.

When results from biodegradation tests simulating the conditions in surface waters are not available, the use of results from various screening tests may be considered. **Table 7** gives a proposal for first order rate constants for surface water to be used in local and especially, regional models, based on the results of screening tests for biodegradability. The proposal is based on general experience in relation to available data on biodegradation half-lives in surface waters of readily and not readily biodegradable substances.

The assigned degradation half-lives of an inherently biodegradable substance of 150 days in surface water (**Table 7**) and 300 – 30,000 days in soil and sediment (**Table 8**) will only affect the predicted regional concentration provided that the residence time of the substance is much larger than the assigned half-life (i.e. only for substances present in soil compartment and sediment).

It is noted that the conditions in laboratory screening tests are very different from the conditions in various environmental compartments. The concentration of the test substance is several orders of magnitude greater in these screening tests than the concentrations of xenobiotic substances generally occurring in the environment and thus the kinetic regimes are significantly different. The temperature is also higher in screening tests than those generally occurring in the environment. Furthermore the microbial biomass is normally lower under environmental conditions than those occurring in these screening tests, especially in the tests for inherent biodegradability. These factors are taken into account in the proposed degradation rates and half-lives in **Tables 7** and **8**.

Table 7 First order rate constants and half-lives for biodegradation in surface water based on results of screening tests on biodegradability [a)]

Test result	Rate constant k (d^{-1})	Half-life (d)
Readily biodegradable	$4.7 \cdot 10^{-2}$	15
Readily, but failing 10-d window [b)]	$1.4 \cdot 10^{-2}$	50
Inherently biodegradable [c)]	$4.7 \cdot 10^{-3}$	150
Not biodegradable	0	∞

Notes to Table 7:

a) For use in exposure models these half-lives do not need to be corrected for different environmental temperatures.

b) The 10-day time window concept does not apply to the MITI test. The value obtained in a 14-d window is regarded as acceptable in the Closed Bottle method, if the number of bottles that would have been required to evaluate the 10-d window would cause the test to become too unwieldy.

c) Only those inherently degradable substances that fulfil the criteria described in note b) to Table 6 above. The half-life of 150 days reflects a present "best expert judgement".

The general experience is that a substance passing a test for ready biodegradability may under most environmental conditions be rapidly degraded and the estimated half-lives for such substances (cf. **Table 7**) should therefore be regarded as being in accordance with “the realistic worst-case concept”. An OECD guidance document for classification of chemicals hazardous for the aquatic environment (OECD, 2001c) contains a chapter on interpretation of degradation data. Even though this guidance relates to hazard classification and not risk assessment, many of the considerations and interpretation principles may also apply in a risk assessment context. One difference is of course that in the risk assessment context not only a categorisation of the substance (i.e. a classification) is attempted, but instead an approximate half-life is estimated.

Another difference is that for risk assessment, the availability of high quality test data is required in virtually all cases and further testing may therefore be required in the case of low quality data.

In distribution models, calculations are performed for compartments each consisting of homogeneous sub-compartments, i.e. surface water containing dissolved organic carbon and suspended matter, sediment containing porewater and a solid phase, and soil containing air, porewater and a solid phase. Since it is assumed that no degradation takes place in the sorbed phase, the rate constant for the surface water, bulk sediment or soil in principle depends on the suspended matter/water, sediment/water or soil/water partition coefficient of the substance. With increasing hydrophobicity (sorption) of the substance, the freely dissolved fraction present in the water phase available for degradation decreases, and therefore the overall rate constant should also decrease. However, for surface waters the influence of sorption is already comprised in the degradation rates when they are determined for bulk water in simulation tests employing the same conditions as in the aquatic environment. Neither is it needed to consider the influence of sorption processes when rate constants are established from screening test results due to the well-established practice to conclude on biodegradability in the environment from such data.

Also for assessment of biodegradation in soil or sediment, data from relevant simulation tests are preferred. Simulation tests such as the OECD 307 "Aerobic and anaerobic transformation in soil" (OECD, 2000b; EU Annex V draft C.23) and the OECD 308 "Aerobic and anaerobic transformation in aquatic sediment systems" (OECD, 2000c; EU Annex V draft C.24) are available. The basis for these methods was initially developed for pesticides, e.g. guidelines of BBA (BBA, 1986; BBA, 1990a) and US EPA. The draft ISO/DIS 14592-1 standard includes an option for determination of biodegradability in a surface water/sediment suspension. Of course this test does not directly simulate the conditions in non-disturbed sediment. The measured half-life in water/sediment tests may be dependent on the relative volume of water and sediment employed in the test.

When such simulation test data are available, the applicability of the results from the tests should be evaluated on a case-by-case basis employing expert judgement when used in a risk assessment.

When no data from tests simulating the conditions in soil or sediment are available, the use of screening test data may be considered. The guidance for use of such data is based on the general recognition that for substances with low Kp values at present not enough empirical data are available to assume some sort of dependence of the soil biodegradation half-life on the solids/water partition coefficient. Nevertheless, for substances with high Kp values there is evidence that some sort of Kp dependence exists. Therefore degradation half-life classes for (bulk) soil, partly based on Kp are presented in **Table 8**. If a half-life from a surface water simulation test is available it may, in a similar manner, form the basis for the establishment of a half-life in soil. The half-lives indicated in the table are considered conservative.

Table 8 Half-lives (days) for (bulk) soil based on results from standardised biodegradation test results

Kp_{soil} * [l · kg^{-1}]	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
≤ 100	30	90	300
>100, ≤ 1000	300	900	3,000
>1000, ≤ 10,000	3,000	9,000	30,000
etc.	etc.	etc.	etc.

* Measured Kp_{soil} values are preferred, but if not available and assuming an EU standard soil these values correspond to log Kow values of 4.4 (Kp_{soil} = 100), 5.7 (Kp_{soil} = 1000), and 6.9 (Kp_{soil} = 10,000) using the TGD QSAR equations for Kp_{soil} as a function of Kow (cf. Chapter 4).

If no aquatic simulation or screening test data are available, a degradation rate for surface water may be established from a result of a simulation test for soil biodegradation. A substance may be considered readily biodegradable if it is ultimately degraded within 28 days in soil with a half-life <16 days, no pre-exposure has taken place and a realistic concentration has been employed (cf. OECD, 2000b).

The following equation can be used to convert DT50 to a rate constant for biodegradation in soil:

$$kbio_{soil} = \frac{\ln 2}{DT50\,bio_{soil}} \tag{29}$$

Explanation of symbols

$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	Table 8
$kbio_{soil}$	first order rate constant for degr. in bulk soil		[d^{-1}]

The extrapolation of results from biodegradation tests to rate constants for sediment is problematic given the fact that sediment in general consists of a relatively thin oxic top layer and anoxic deeper layers. For the degradation in the anoxic layers a rate constant of zero (infinite half-life) can be assumed unless specific information on degradation under anaerobic conditions is available. For the oxic zone, similar rate constants as the ones for soil can be assumed. For the present regional model, a 3 cm thick sediment compartment is assumed with aerobic conditions in the top 3 mm. The sediment compartment is assumed to be well mixed with respect to the substance concentration. This implies that the total half-life for the sediment compartment will be a factor of ten higher than the half-life in soil. The degradation half-life for sediment is given by:

$$kbio_{sed} = \frac{\ln 2}{DT50\,bio_{soil}} \cdot Faer_{sed} \tag{30}$$

Explanation of symbols

$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	Table 8
$Faer_{sed}$	fraction of the sediment compartment that is aerobic	[m^3 · m^{-3}]	0.10
$kbio_{sed}$	first order rate constant for degr. in bulk sediment	[d^{-1}]	

The remarks in the section on soil biodegradation regarding use of half-lives derived in surface water simulation tests may also apply for sediments.

2.3.6.6 Overall rate constant for degradation in surface water

In surface water, the substance may be transformed through photolysis, hydrolysis, and biodegradation. For calculation of the PECregional, the rate constants for these processes can be summed into one, overall degradation rate constant. It should be noted that different types of degradation (primary and ultimate) are added. This is done for modelling purposes only. It should also be noted that measurements on one degradation process might in fact already include the effects of other processes. For example, hydrolysis can occur under the conditions of a biodegradation test or a test of photodegradation, and so may already be comprised by the measured rate from these tests. In order to add the rates of different processes, it should be determined that the processes occur in parallel and that their effects are not already included in the rates for other processes. If exclusion of hydrolysis from the other degradation rates cannot be confirmed its rate constant should be set to zero. The equation below relates to primary degradation. If the primary degradation is not the rate-limiting step in the total degradation sequence and degradation products accumulate, then also the degradation product(s) formed in the particular process (e.g. hydrolysis) should be assessed. If this cannot be done or is not practical, the rate constant for the process should be set to zero.

$$kdeg_{water} = khydr_{water} + kphoto_{water} + kbio_{water} \quad (31)$$

Explanation of symbols

$khydr_{water}$	first order rate constant for hydrolysis in surface water	[d^{-1}]	eq. (26)
$kphoto_{water}$	first order rate constant for photolysis in surface water	[d^{-1}]	eq. (27)
$kbio_{water}$	first order rate constant for biodegradation in surface water	[d^{-1}]	Table 7
$kdeg_{water}$	total first order rate constant for degradation in surface water	[d^{-1}]	

2.3.7 Elimination processes prior to the release to the environment

2.3.7.1 Wastewater treatment

In this section, the following parameters are derived:

- emission from a sewage treatmentplant to air;
- concentration in sewage sludge;
- concentration in effluent of a sewage treatment plant;
- PEC for microorganisms in a sewage treatment plant.

Elimination refers to the reduction in the concentration of substances in gaseous or aqueous discharges prior to their release to the environment. Elimination from the water phase may occur by physical as well as chemical or biochemical processes. In a sewage treatment plant (STP), one of the main physical processes is settling of suspended matter which will also remove adsorbed material. Physical processes do not degrade a substance but transfer it from one phase to another e.g. from liquid to solid. In the case of volatile substances, the aeration process will

enhance their removal from the water phase by "stripping" them from the solid/liquid phases to the atmosphere. Substances may be removed from exhaust gaseous streams by scrubbing e.g. by adsorption on a suitable material or by passing through a trapping solution.

Wastewater treatment

One of the critical questions to answer in determining the PEC for the aquatic environment is whether or not the substance will pass through a wastewater treatment plant and if yes, through which kind of treatment plant before being discharged into the environment. The situation in the Member States concerning percentage connection to sewage works is quite diverse (see Appendix XII). The percentage connection rate across the Community is subject to improvement due to the implementation of the Urban Waste Water Treatment Directive (UWWTD, 91/271/EEC). This directive requires Member States (via transposition into national legislation) to ensure that wastewater from all agglomerations of > 2,000 population equivalents is collected and treated minimally by secondary treatment. The time limit for implementation of the directive is 31/12/98, 31/12/2000 or 31/12/2005 dependent on the size of the agglomeration and the sensitivity of the receiving water body. An interim figure of 80% connection to wastewater treatment is proposed for the regional standard environment. This value is thought to be representative for the actual situation in large urban areas at the time of revision of the TGD. Article 6 of the UWWTD allows Member States to declare non sensitive areas for which discharged wastewater from agglomerations between 10,000 and 150,000 population equivalents, which are located at the sea and from agglomerations between 2,000 and 10,000 population equivalents located at estuaries does not have to be treated biologically but only mechanically (primary treatment). It is notable that 4 Member States have applied this article, corresponding to < 9% of the organic load (in terms of population equivalents).

The situation with respect to wastewater treatment at industrial installations is less clear. It may be assumed that many of the larger industrial installations are either connected to a municipal wastewater treatment plant or have treatment facilities on site. In many cases, these treatment plants are not biological treatment plants but often physico-chemical treatment plants in which organic matter is flocculated by auxiliary agents e.g. by iron salts followed by a sedimentation process resulting in a reduction of organic matter measured as COD of about 25-50%.

In the present document, the above-described situation is taken into account as follows:

- on a local scale, it is assumed that wastewater will pass through a STP before being discharged into the environment. Nevertheless, for the largest PEClocal in surface water, it is necessary to determine an aquatic PEClocal assuming that no sewage treatment will take place. This value should be determined in addition to the normal PEC that assumes sewage treatment to flag for possible local problems (this PEC/PNEC ratio will not normally be used in risk characterisation). The alternative/additional PEC can be used to explore the possibility of environmental impact in regions or industrial sectors where percentage connection to sewage works is currently low, so as to give indications to local authorities for needs of possible local risk reductions. The PEC without considering a STP-treatment will not be used in the exposure assessment, unless the substance considered has a specific use category where direct discharge to water is widely practised;
- for a standard regional scale environment (definition see Section 2.3.8.1) it is assumed that 80% of the wastewater is treated in a biological STP and the remaining 20% released directly into surface waters (although mechanical treatment has some effect on eliminating organic matter, this is neglected because on the other hand stormwater overflows usually result in direct discharges to surface water even in the case of biological treatment. It is

assumed that these two adverse effects compensate each other more or less with regard to the pollution of the environment).

The degree of removal in a wastewater treatment plant is determined by the physico-chemical and biological properties of the substance (biodegradation, adsorption onto sludge, sedimentation of insoluble material, volatilisation) and the operating conditions of the plant. As the type and amount of data available on degree of removal may vary, the following order of preference should be considered:

Measured data in full scale STP

The percentage removal should preferably be based upon measured influent and effluent concentrations. As with measured data from the environment, the measured data from STPs should be assessed with respect to their adequacy and representativeness.

Consideration must be given to the fact that the effectiveness of elimination in treatment plants is quite variable and depends on operational conditions, such as retention time in the aeration tank, aeration intensity, influent concentration, age and adaptation of sludge, extent of utilisation, rainwater retention capacity, etc. The data may be used provided that certain minimum criteria have been met, e.g. the measurements have been carried out over a longer period of time. Furthermore, consideration should be given to the fact that removal may be due to stripping or adsorption (not degradation). In case no mass balance study has been performed, the percentage of transport to air or sludge should be estimated, e.g. by scaling the fractions to air and sludge from the tables in Appendix II to the measured removal.

Data from dedicated STPs should be used with caution. For example, when measured data are available for highly adapted STPs on sites producing high volume site-limited intermediates, these data should only be used for the assessment of this specific use category of the substance.

Simulation test data

Simulation testing is the examination of the potential of a substance to biodegrade in a laboratory system designated to represent either the activated sludge-based aerobic treatment stage of a wastewater treatment plant or other environmental situations, for example a river. The wastewater treatment process can be studied in the laboratory by, e.g., the updated OECD guideline on simulation testing of aerobic sewage treatment (OECD, 2001b) or the older Coupled Units Test (OECD, 1981b). Removability is determined by monitoring the changes in DOC (Dissolved Organic Carbon) and/or COD (Chemical Oxygen Demand). A number of guidelines have recently been prepared, e.g. ISO/DIS 14952-1, draft OECD (2001d), OECD 307 (soil, 2000b), draft EU Annex V C.23, OECD 308 (sediment, 2000c), draft EU Annex V C.24.

The Coupled Units Test is not suitable for adsorptive, poorly water-soluble and volatile substances because it is an open test and is only based on DOC analysis. Since, in addition, it is possible that adsorptive or volatile metabolites may be formed during biological degradation, this test cannot differentiate between biological degradation and other elimination processes. Investigations with a closed vessel version of the Coupled Units Test using radioactively labelled substances have been performed which would allow a determination of the complete mass balance and would also be suitable for volatile or adsorptive substances. However, there is no international standard method available for this modified test.

There is insufficient information available on the applicability of elimination data from the laboratory test to the processes of a real sewage plant. The results can be extrapolated to

degradation in the real environment only if the concentrations that were used in the test are in the same order of magnitude as the concentrations that are to be expected in the real environment. If this is not the case, extrapolation can seriously overestimate the degradation rates especially when the extrapolation goes from high to low concentrations. If concentrations are in the same order of magnitude then the results of these tests can be used quantitatively to estimate the degree of removal of substances in a mechanical-biological STP.

If a complete mass balance is determined, the fraction removed by adsorption and stripping should be used for the calculation of sludge and air concentrations. In case no mass balance study has been performed, the percentage of transport to air or sludge should be estimated for example by using the tables in Appendix II.

Modelling STP

If there are no measured data available, the degree of removal can be estimated by means of a wastewater treatment plant model using log Kow (Koc or more specific partition coefficients can also be used; see Section 2.3.5), Henry's Law constant and the results of biodegradation tests as input parameters. However, it should be remembered that the distribution behaviour of transformation products is not considered by this approach. It is proposed to use in the screening phase of exposure assessment a revised version of the sewage treatment plant model SimpleTreat (Struijs et al., 1991). This model is a multi-compartment box model, calculating steady-state concentrations in a sewage treatment plant, consisting of a primary settler, an aeration tank and a liquid-solid separator. With SimpleTreat, the sewage treatment plant is modelled for an average size treatment plant based on aerobic degradation by active sludge, and consisting of 9 compartments (see **Figure 6**). Depending on the test results for ready and/or inherent biodegradability of a substance, specific first order biodegradation rate constants are assigned to the compound. An improved process formulation for volatilisation from the aeration tank, which is also applicable to semi-volatile substances (Mikkelsen, 1995), has been incorporated in the revised version.

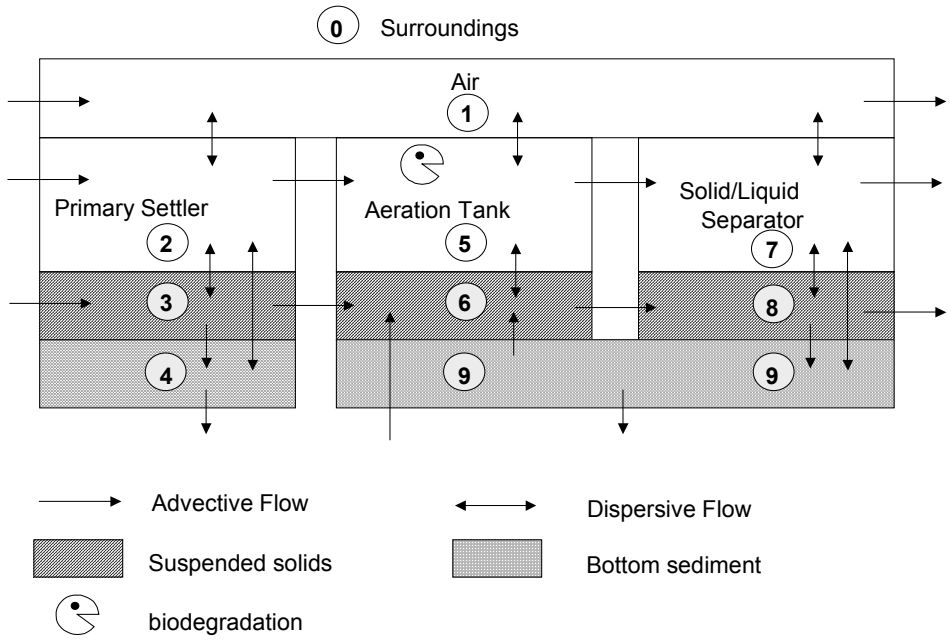

Figure 6 Schematic design of the sewage treatment plant model Simple Treat

For the purpose of modelling a STP, the rate constants presented in **Table 6** have been derived from the biodegradation screening tests. The modelling results from SimpleTreat using these first-order rate constants of 0, 0.1, 0.3 and 1 h-1 are tabulated in Appendix II. It contains relative emission data pertaining to air, water, and sludge as a function of Henry's Law constant and log Kow for the different biodegradation categories, according to **Table 6**. If no specific measured biodegradation rate data are available for the particular substance, the tabulated values from Appendix II should be used.

Typical characteristics of the standard sewage treatment plant are given in **Table 9**. The amount of surplus sludge per person equivalent and the concentration of suspended matter in influent are taken from SimpleTreat (run at low loading rate).

These values are the same as applied to derive the tables in Appendix II. At a higher tier in the risk assessment process more specific information on the biodegradation behaviour of a substance may be available. In order to take this information into account a modified version of the SimpleTreat model may be used. In this version the following scenarios are optional:

- temperature dependence of the biodegradation process;
- degradation kinetics according to the Monod equation;
- degradation of the substance in the adsorbed phase;
- variation in the sludge retention time;
- not considering a primary settler.

Table 9 Standard characteristics of a municipal sewage treatment plant

Parameter	Symbol	Unit	Value
Capacity of the local STP	$CAPACITY_{stp}$	[eq]	10,000
Amount of wastewater per inhabitant	WASTEWinhab	$[l \cdot d^{-1} \cdot eq^{-1}]$	200
Surplus sludge per inhabitant	SURPLUSsludge	$[kg \cdot d^{-1} \cdot eq^{-1}]$	0.011
Concentration susp. matter in influent	$SUSPCONC_{inf}$	$[kg \cdot m^{-3}]$	0.45

Consultation of the tables in Appendix II gives the following input-output parameters:

Input

HENRY	Henry's law constant	$[Pa \cdot m^3 \cdot mol^{-1}]$	eq. (21)
Kow	octanol-water partitioning coefficient	[-]	data set
$kbio_{stp}$	first-order rate constant for biodegradation in STP	$[d^{-1}]$	Table 6

Output

$Fstp_{air}$	fraction of emission directed to air by STP	[-]
$Fstp_{water}$	fraction of emission directed to effluent by STP	[-]
$Fstp_{sludge}$	fraction of emission directed to sludge by STP	[-]

Calculation of the STP influent concentration

For local scale assessments, it is assumed that one point source is releasing its wastewater to one STP. The concentration in the influent of the STP, i.e. the untreated wastewater, can be calculated from the local emission to wastewater and the influent flow to the STP. The influent flow equals the effluent discharge.

$$Clocal_{inf} = \frac{Elocal_{water} \cdot 10^6}{EFFLUENT_{stp}} \tag{32}$$

Explanation of symbols

$Elocal_{water}$	local emission rate to (waste) water during episode	$[kg \cdot d^{-1}]$	eq. (5)
$EFFLUENT_{stp}$	effluent discharge rate of STP	$[l \cdot d^{-1}]$	eq. (34)
$Clocal_{inf}$	concentration in untreated wastewater	$[mg \cdot l^{-1}]$	

Calculation of the STP-effluent concentration

The fraction of the substance reaching the effluent of the STP is tabulated in Appendix II. The concentration of the effluent of the STP is given by the fraction directed to effluent and the concentration in untreated wastewater as follows:

$$Clocal_{eff} = Clocal_{inf} \cdot Fstp_{water} \tag{33}$$

Explanation of symbols

$Clocal_{inf}$	concentration in untreated wastewater	[mg · l^{-1}]	eq. (32)
$Fstp_{water}$	fraction of emission directed to water by STP	[-]	App. II
$Clocal_{eff}$	concentration of substance in the STP effluent	[mg · l^{-1}]	

If no specific data are known, $EFFLUENT_{stp}$ should be based on an averaged wastewater flow of 200 l per capita per day for a population of 10,000 inhabitants (see **Table 9**):

$$EFFLUENT_{stp} = CAPACITY_{stp} \cdot WASTEWinhab \quad (34)$$

Explanation of symbols

$CAPACITY_{stp}$	capacity of the STP	[eq]	Table 9
WASTEWinhab	sewage flow per inhabitant	[l · d^{-1} · eq^{-1}]	Table 9
$EFFLUENT_{stp}$	effluent discharge rate of STP	[l · d^{-1}]	

For calculating the PEC in surface water without sewage treatment, the fraction of the emission to wastewater, directed to effluent ($Fstp_{water}$) should be set to 1. The fractions to air and sludge ($Fstp_{air}$ and $Fstp_{sludge}$ resp.) should be set to zero.

Calculation of the emission to air from the STP

The indirect emission from the STP to air is given by the fraction of the emission to wastewater, which is directed to air:

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water} \quad (35)$$

Explanation of symbols

$Fstp_{air}$	fraction of the emission to air from STP	[-]	App. II
$Elocal_{water}$	local emission rate to water during emission episode	[kg · d^{-1}]	eq. (5)
$Estp_{air}$	local emission to air from STP during emission episode	[kg · d^{-1}]	

Calculation of the STP sludge concentration

The concentration in dry sewage sludge is calculated from the emission rate to water, the fraction of the emission sorbed to sludge and the rate of sewage sludge production:

$$C_{sludge} = \frac{Fstp_{sludge} \cdot Elocal_{water} \cdot 10^6}{SLUDGERATE} \quad (36)$$

Explanation of symbols

$Elocal_{water}$	local emission rate to water during episode	[kg · d^{-1}]	eq. (5)
$Fstp_{sludge}$	fraction of emission directed to sludge by STP	[-]	App. II
SLUDGERATE	rate of sewage sludge production	[kg · d^{-1}]	eq. (37)
C_{sludge}	concentration in dry sewage sludge	[mg · kg^{-1}]	

The rate of sewage sludge production can be estimated from the outflows of primary and secondary sludge as follows:

$$SLUDGERATE = \frac{2}{3} \cdot SUSPCONC_{inf} \cdot EFFLUENT_{stp} + SURPLUSsludge \cdot CAPACITY_{stp} \qquad (37)$$

Explanation of symbols

$SUSPCONC_{inf}$	concentration of suspended matter in STP influent	[kg · m^{-3}]	Table 9
$EFFLUENT_{stp}$	effluent discharge rate of STP	[m^3 · d^{-1}]	eq. (34)
SURPLUSsludge	surplus sludge per inhabitant equivalent	[kg · d^{-1} · eq^{-1}]	Table 9
$CAPACITY_{stp}$	capacity of the STP	[eq]	Table 9
SLUDGERATE	rate of sewage sludge production	[kg · d^{-1}]	

Anaerobic degradation may lead to a reduction of the substance concentration in sewage sludge during digestion. This is not yet taken into account.

Calculation of the STP concentration for evaluation of inhibition to microorganisms

As explained above in the section on STP modeling, the removal of a chemical in the STP is computed from a simple mass balance. For the aeration tank this implies that the inflow of sewage (raw or settled, depending on the equipment with a primary sedimentation tank) is balanced by the following removal processes: degradation, volatilization and outflow of activated sludge into the secondary settler. Activated sludge flowing out of the aeration tank contains the chemical at a concentration similar to the aeration tank, which is the consequence of complete mixing. It consists of two phases: water, which is virtually equal to effluent flowing out of the solids-liquid separator (this is called the effluent of the STP), and suspended particles, which largely settle to be recycled into the aeration tank. Assuming steady state and complete mixing in all tanks (also the aeration tank), the effluent concentration approximates the really dissolved concentration in activated sludge. It is assumed that only the dissolved concentration is bioavailable, i.e. the actual concentration to which the microorganisms in activated sludge are exposed. For the risk characterisation of a substance upon microorganisms in the STP, it can therefore be assumed that homogeneous mixing in the aeration tank occurs which implies that the dissolved concentration of a substance is equal to the effluent concentration:

$$PEC_{stp} = Clocal_{eff} \qquad (38)$$

Explanation of symbols

$Clocal_{eff}$	total concentration of substance in STP effluent	[mg · l^{-1}]	eq. (33)
PEC_{stp}	PEC for microorganisms in the STP	[mg · l^{-1}]	

In the case of intermittent release the situation is much more complex. During an interval shorter than several sludge retention times (SRT), presumably a small portion of the competent microorganisms will remain in the system. If the interval between two releases is shorter than one month (three times an average SRT), adaptation of the activated sludge is maintained resulting in rapid biodegradation when a next discharge enters the STP. In line with Section 2.3.3.4. such a situation is not considered as an intermittent release and the PEC_{STP} can still be considered equal to $Clocal_{eff}$. After longer intervals the specific bacteria that are capable to biodegrade the compound, may be completely lost.

If the activated sludge is de-adaptated, the concentration in the aeration tank may increase during the discharge period. In that case the concentration in influent of the STP is more representative for the PEC for microorganisms:

$$PEC_{stp} = Clocal_{inf} \quad (39)$$

Explanation of symbols

$Clocal_{inf}$	total concentration of substance in STP influent	$[mg \cdot l^{-1}]$	eq. (32)
PEC_{stp}	PEC for microorganisms in the STP	$[mg \cdot l^{-1}]$	

However, it needs to be noted that when the discharge period is shorter than the hydraulic retention time of the aeration tank (7-8 h), the maximum concentration in the effluent will be lower than the initial concentration at the discharge, due to peak dispersion, dilution and sorption in the sewer system, the primary settler and the activated sludge process. It is estimated that this maximum concentration will be at least a factor of three lower than the initial concentration. Whether or not this correction factor must be applied needs to be decided on a case-by-case basis. For such short emission periods care must be taken that the emission rates are in fact calculated over the actual emission period (as $kg \cdot h^{-1}$) and not averaged out over one day.

The choice of using the effluent concentration is also reflected in the choice of the assessment factors used for deriving a PNEC for the STP microorganisms. In modern wastewater treatment plants with a denitrification stage, an additional tank is normally placed at the inlet of the biological stage. As the main biological degradation processes are taking place in the second stage, the microbial population in the denitrification tank is clearly exposed to higher concentrations of the substance as compared to the effluent concentration. As the technical standard of the STPs improves, this will have to be addressed in this assessment scheme in the near future.

2.3.7.2 Waste disposal, including waste treatment and recovery

This section contains preliminary guidance on how to identify specific concerns related to the waste life-cycle stage of a substance. Since representative data on waste disposal operations in Europe are not available at this stage, qualitative aspects are addressed rather than quantitative emission modelling.

Elimination refers to degradation (organic substances), transformation and reduced mobility of organic and inorganic substances in waste. Elimination can result from physical processes and degradation (biotic and abiotic). Waste incineration is targeted at the thermal-oxidative destruction of organic substances. Controlled landfill aims to slow down or even prevent the

release of substances from waste to the environment. Substances under assessment may occur in various types of waste streams at the end of their service life, depending on the product type of which they are a component e.g.:

- components in consumer products and articles may end up in municipal waste;
- components in construction and building material including paints and sealants may end up in construction waste;
- spent processing fluids (solvents, lubricants, dyestuffs, cleaners) from industry may be disposed of as hazardous waste;
- discarded electric/electronic equipment, vehicles and machinery at the end of their service life may undergo mechanical separation of metals from plastic and other components. The non-metal compounds may be disposed off as manufacturing waste, e.g. shredder material.

To assess the waste-related risk of a substance, a translation from substance to use category (Appendix I) and further to product category (no European system yet existing) is needed, as well as a translation from product category to waste category (Draft European Commission proposal 2001, or European Waste Catalogue) and further to waste management/treatment category (see Directive 75/442/EEC, Appendix IIA and IIB).

In estimating the volume of a substance that enters a certain waste management system it is important to use the knowledge on the products in which the substance occur as far as possible. In many cases a certain waste management is directly related to the product and product use. Only in cases and for the fraction of the total substance volume where such information cannot be made available the more generic translation from use category to product to waste category and to waste management should be performed (see e.g. Danish EPA, 2001).

Waste management practise varies considerably among different countries and regions in the EU, so in determining the realistic worst case, due considerations should be given whether incineration, direct landfilling (e.g. for organic substances) or recovery should be considered as the realistic worst case. Unless more detailed information is available on waste management of specific product types containing the substance of concern, two alternative scenarios may be explored as a first approach assuming either 100% incineration or 100% landfilling. Both these conditions are relevant for different parts of the EU. As a consequence of this sensitivity analysis any risk indication may refer to a certain waste management practice rather than to an average waste management in a generic EU region.

Certain groups of products may be separately collected or removed from municipal waste streams prior to final disposal (e.g. packaging material, batteries, paper, electronic waste) or usually do not occur in waste streams from households (e.g. paints and varnishes in construction waste and industrial waste from shredder installations). However, the extent of waste separation and specific waste management schemes may largely differ among member states and regions. Thus, the realistic worst case needs to be defined on a case by case basis, taking into account i) which type of waste management (specialised or mixed disposal) would lead to higher emissions and ii) what fraction of the substance enters into this type of waste management.

Municipal waste incineration

Waste incineration aims at the thermal-oxidative destruction of organic substances. It is assumed that waste incinerators operated at ‘best available technology’ level achieve a high level of destruction and that residual releases of the organic substance under risk assessment are negligible. Nevertheless, products of incomplete combustion or substances formed by catalytic

de novo synthesis may occur. Both types of releases are a result of the technical conditions (temperature, turbulence and time) of the waste incineration rather than caused by specific types of chemical substances and they are as such not covered by the risk assessment. An exception from this general rule may be waste streams, containing organobromine substances or other halogenated hydrocarbons.

It is assumed that waste incineration processes operated in compliance with EU Directive 89/429/EC and 94/67/EC (or with Directive 2000/76/EC) would lead to sufficient destruction of organic substances in the waste stream. In special cases it may be known that incineration conditions differ from 'best available technology' conditions and in that case information on melting and boiling point as well as on thermal stability may be used to assess whether complete destruction of the substance of concern can be expected. Even though waste incinerators may be regarded as a major source of PCDD/PCDFs in Europe, the potential risk is related to the installation rather than the substance under assessment.

While organic substances are destroyed in the municipal incinerator, inorganic substances such as metals will be distributed among various incineration residues or emitted to the atmosphere. Typical range of concentration in incineration residues from incineration of municipal waste can be determined, based on modelling or measurements (e.g. Danish EPA, 2001). The distribution pattern is different for each inorganic substance, depending on its physico-chemical properties, the gas cleaning technology and the operation conditions. For metals emissions to the atmosphere with the flue gas may vary from less than 0.1 % to 15% of the input depending on the substance properties and the employed flue gas treatment technology (Danish EPA, 2001).

The main emissions source related to waste incinerator residues is leaching from landfilled or from recovered residues. The high content of salts and metals in bottom ashes and in flue gas cleaning products suggest that these residues could potentially sustain leaching of salts and metals for a prolonged period of time (compared to the general time frame within risk assessment) at elevated concentrations compared to background concentrations in surface and groundwater. However, the magnitude of the long-term releases depends on processes both governing and limiting the leaching potential and is therefore uncertain. As a first cautious approach leaching tests may be used (c.f. Danish EPA, 2001) whereas monitoring data regarded as representative may be used to modify such an estimation. Concerns related to leaching from incineration residues are dependent on the present and future intended use of the residues i.e. concerns are related to a general waste management issue rather than to a substance specific risk assessment.

Releases from municipal landfills

Modern landfills aim to prevent uncontrolled emissions and reduce emissions of waste compounds and degradation products into the environment for a number of decades. The principal means for emission control are:

- a top layer to prevent inflow of rain water;
- a bottom liner to prevent leaching to groundwater;
- leachate treatment;
- active collection of landfill gas (in case of organic landfills).

The operation and construction of landfills varies throughout the EU. Even within individual Member States different types of landfills exist. Representative data on EU level are not yet available.

Emission control measures and emission rates change over the three principal life stages of a landfill: filling (e.g. 2 years), active metabolism (e.g. 25 years), passive stage but still functioning emission control (e.g. 30 years). Organic landfills and inorganic landfills (e.g. for construction waste) largely differ from each other, with regard to the relevance of gas as a transport medium and the adsorptive capacity of the landfilled material.

After the technical lifetime of the landfill (e.g. about 60 years) a low but long lasting flow of non-degraded substances into the environment will take place.

The main routes of emissions of substances from landfills are identified as leaching with water, transport with landfill gas, and diffusion to the atmosphere. The most important route of emission depends on the properties of the substance. Most metals will for example almost exclusively leave the landfill with the leachate whereas transport with landfill gas may be important for some organic substances.

For organic substances the emissions will be highly influenced by the degree of degradation of the substance in the landfill and information on the anaerobic degradability is needed. Such information may in many cases be obtained from simple screening or laboratory tests. In utilising such data, however, it is important to note that environmental conditions in landfills may very well differ from conditions in these simple tests. If results from tests at more realistic conditions are available they should be used.

Landfill leachates may be treated in a sewage treatment plant and the risk from the substance to the STP microorganisms may need to be assessed on a case-by-case basis.

In general measured long-term emission data of sufficient analytical quality and knowledge of chemical composition of the landfilled waste are lacking. Therefore, the expected fate of a substance going into a landfill is largely based on modelling. Examples of such models can be found in Van der Poel (1999) and Danish EPA (2001).

Sensitivity analysis of such models provides useful insight in landfill emission patterns depending on substance properties and assumptions on landfill management practices. Substances with different properties may reach their maximum emission rates at different time of the landfill lifecycle. An example of a sensitivity analysis with respect to substance properties is described in Danish EPA (2001) for the landfill chemical fate model MOCLA. This analysis on non-degradable substances indicates:

- at which point in time the maximum emission (flux) may occur (e.g. at the end of active phase);
- what fraction of the input that may be emitted with gas or leachate (e.g. less that 0.1% to more than 10% of annual input);
- how the emission rate may be influenced by a low carbon content in the landfill, the absence of a bottom liner or absence of active gas collection.

Separation of waste components and recovery

Pre-treatment is often carried out after collection of articles or chemical products at the end of their service life, to separate valuable waste compounds from compounds to be finally disposed of. If such treatment steps are carried out as an integrated element in processing and use, the

emission should be assessed in life-cycle stage 3 (industrial/professional use, e.g. paper production or photographic processing, metal production in secondary smelters).

If, however, separation and recovery is carried out in specific types of installations it may be necessary to characterise the emission from this stage of the life-cycle. Certain types of such installations have a wide-spread occurrence in Europe and may contribute with a relevant share of emission, e.g.: i) mechanical extraction of metal scrap from old vehicles or electric household equipment, ii) chemical-physical treatment of spent processing fluids from metal processing (e.g. cutting fluids, electroplating fluids) and iii) thermal treatment to remove organic components from metals or mineral fractions (e.g. cement kilns).

Whether or not the emission from such recovery operations (including pre-treatment) would contribute with relevant emissions must be evaluated on a case-by-case basis.

2.3.8 Calculation of PECs

In this section, the following parameters are derived:

- local PECs for all environmental compartments;
- regional PECs for all environmental compartments.

2.3.8.1 Introduction

In the following sections guidance is given for the calculation of the PEClocal for each compartment. In Section 2.3.8.7, the calculation of regional steady-state concentrations (PECregional) in each compartment is presented. **Table 10** presents an overview of the PECs that need to be estimated.

In defining the standard environments a number of assumptions have to be made with respect to scale and time. These are summarised briefly here. More detail is given in the relevant sections.

- the concentration in surface water ($PEClocal_{water}$) is in principle calculated after complete mixing of the effluent outfall. Because of the short time between effluent discharge and exposure location, dilution will usually be the dominant "removal" process. Therefore, degradation in surface waters, volatilisation from the water body, and sedimentation are not normally taken into account as removal processes. A standard dilution factor is used. To allow for sorption, a correction is made to take account of the fraction of substance that is adsorbed to suspended matter. The resulting dissolved concentration is used for comparison with $PNEC_{water}$ (Section 2.3.8.3). The concentration in sediment is calculated at the same location. For exposure of aquatic organisms, having a relatively short lifespan, the concentration during an emission episode is calculated. For indirect exposure of humans and predatory birds and mammals, annual averages are used, being more appropriate with respect to chronic exposure;
- the concentration in soil ($PEClocal_{soil}$) is calculated as an average concentration over a certain time-period in agricultural soil, fertilised with sludge from a STP and receiving continuous aerial deposition from a nearby point source (Section 2.3.8.5) (production/processing site and STP aeration tank). Two different soil types are distinguished: arable land and grassland, which differ in the amount of sludge applied, and the mixing depth. For the terrestrial ecosystem, the concentration is averaged over 30 days, for human indirect exposure a period of 180 days is used. The concentration in groundwater is calculated below this agricultural area;

- the concentration in air ($PEClocal_{air}$) is calculated as an average concentration at 100 meters from the source. This distance is assumed to be representative for the average size of an industrial site. The concentration in air is used for exposure of humans, therefore, an annual average concentration is calculated. Deposition is calculated as an average for a circle around the source with a radius of 1000 m, which is supposed to represent the local agricultural area (Section 2.3.8.2). Deposition is used as input for the soil module, annual average deposition fluxes are used;
- the regional standard environment is assumed to be highly industrialised, relatively small but densely populated; the size is 200·200 km with 20 million inhabitants. It is assumed that 10% of the European production takes place within this area (Section 2.3.8.7). Emissions are assumed to be a continuous and diffuse flux into the environment.

Further guidance on the estimation of releases during the service life of articles and the waste life stage is described in Sections 2.3.3.5 and 2.3.3.6/2.3.7.2 respectively. Other pathways than those described, like deposition from air to surface waters, could be of relevance. No guidance for those pathways is currently available. Guidance on risk assessment of the marine environment is presented in Chapter 4.

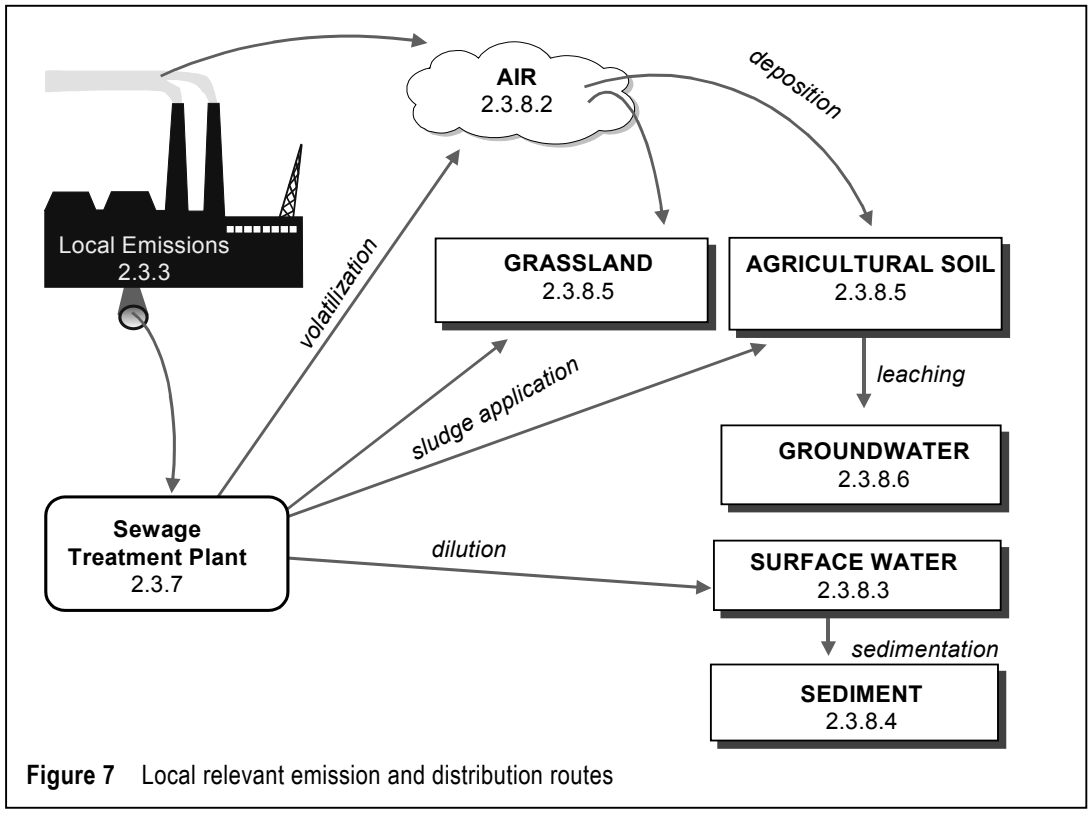

Figure 7 Local relevant emission and distribution routes

Figure 7 shows the relationship between the local emission routes and the subsequent distribution processes, which may be relevant for the different environmental compartments. For each compartment, specific fate and distribution models are applied.

On the regional scale the region under consideration is viewed as a box, consisting of several, homogeneous compartments. All flows of the substance between the different compartments (and with the outside world) are quantified. More specific information can be found in Section 2.3.8.7.

Table 10 Overview of different exposure scenarios and the respective PECs

Target	Medium of exposure	Exposure scenario				Section
		regional	Section	local		
Aquatic com-partment	surface water	steady-state concentration in surface water	2.3.8.7	concentration during emission period taking into account dilution, sorption, and, if relevant, sedimentation, volatilisation and degradation		2.3.8.3
	sediment	steady-state concentration in sediment		equilibrium concentration in freshly deposited sediment, related to the local surface water concentration		2.3.8.4
Terrestrial compartment	agricultural soil	steady-state concentration in agricultural soil		concentration in agricultural soil averaged over 30 days, fertilised with STP sludge over 10 years and receiving input through continuous aerial deposition		2.3.8.5
	ground water	steady-state concentration in groundwater under agricul-tural soil		concentration in groundwater under agricultural soil.		2.3.8.6
Air compartment	air	steady-state concentration in air		concentration in air, at 100 m from point source or STP		2.3.8.2
Microorganisms	STP aeration tank	-	-	concentration during emission period		2.3.7

2.3.8.2 Calculation of PEClocal for the atmosphere

In this section, the following parameters are derived:

- local concentration in air during emission episode;
- annual average local concentration in air;
- total deposition flux (annual average).

The air compartment receives its input from direct emission to air, and volatilisation from the sewage treatment plant. The most important fate processes in air, are schematically drawn in **Figure 8**.

PEClocal for air cannot be compared with the PNEC for air because the latter is usually not available. The PEClocal for air is used as input for the calcu-lation of the intake of substances through inhalation in the indirect exposure of humans. Deposition fluxes are used as input for the calculation of PEClocal in soil. Therefore, both deposition flux and concentration are calculated as annual average values.

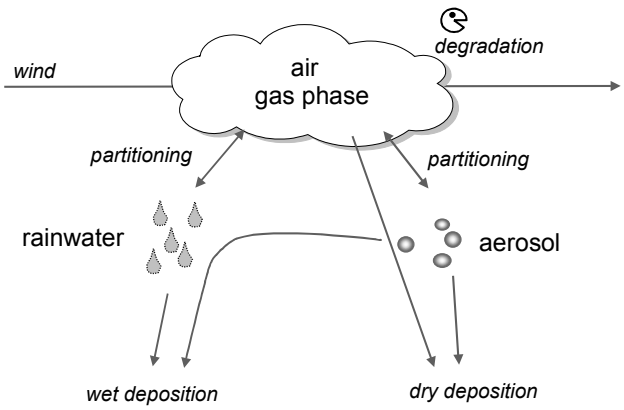

Figure 8 Fate processes in the air compartment

Many air models are available that are highly flexible and can be adjusted to take specific information on scale, emission sources, weather conditions etc. into account. For new substances, as well as very often for existing substances, this type of information is normally not available. Hence a standardised exposure assessment is carried out making a number of explicit assumptions and using a number of fixed default parameters. The gaussian plume model OPS, as described by Van Jaarsveld (1990) is proposed using the standard parameters as described by Toet and de Leeuw (1992). These authors used the OPS model and carried out a number of default calculations in order to describe a relationship between the basic characteristics of substances (vapour pressure and Henry's Law constant) and the concentration in air and deposition flux to soil near to a point source. The following assumptions/model settings are made:

- realistic average atmospheric conditions are used, obtained from a 10-year data set of weather conditions for The Netherlands;
- transport of vaporised and aerosol-bound substances is calculated separately. The partitioning between gas and aerosol is determined by means of the equation of Junge (see equation (19));
- the atmospheric reaction rate is set at a fixed value of 5% per hour. However, on the spatial scale that is regarded (i.e. a distance of 100 m from the source), atmospheric reactions do not play any role in the removal of the substance (even at very high reaction rates) (Toet and De Leeuw, 1992);
- losses due to deposition are neglected for estimation of the concentration and deposition fluxes at this short distance from the source;

- assumed source characteristics are:

- source height: 10 meters, representing the height of buildings in which production, processing or use take place;
- heat content of emitted gases: 0; this assumes there is no extra plume rise caused by excess heat of vapours compared to the outdoor temperature;
- source area: 0 meter; representing an ideal point source which is obviously not always correct but which is an acceptable choice;

- calculated concentrations are long-term averages.

The concentration in air at a distance of 100 meters from the point source is estimated. This distance is chosen to represent the average distance between the emission source and the border of the industrial site. The deposition flux of gaseous and aerosol-bound substances is estimated analogous to the estimation of atmospheric concentrations by means of an estimation scheme and with help of the OPS model. The deposition flux to soil is averaged over a circular area around the source, with a radius of 1000 m to represent the local agricultural area. Deposition velocities are used for three different categories:

- dry deposition of gas/vapour: estimated at 0.01 cm/s;
- wet deposition of gas/vapour: determined with the OPS model;
- dry and wet deposition of aerosol particles; determined within the OPS model using an average particle size distribution.

Based on the assumptions and model settings as listed above, calculations with the original OPS-model were performed for both gaseous and aerosol substances (Toet and de Leeuw, 1992). These calculations were only carried out for a source strength of 1 g/s, as it was proven that concentrations and deposition fluxes are proportional to the source strength. From these calculations it was concluded that local atmospheric concentrations are largely independent of the physical-chemical properties of the compounds. Hence, once the emission from a point source is known, the concentration at 100 meter from the source can be estimated from a simple linear relationship.

In the calculation of PEClocal for air both emission from a point source as well as the emission from a STP is taken into account. The concentration on the regional scale (PECregional) is used as background concentration and therefore, summed to the local concentration. The STP is assumed as a point source and the concentration of the chemical is calculated at a 100 m distance from it. The maximum from the two concentrations (direct and via STP) is used as the PEClocal:

$$Clocal_{air} = \max\left(Elocal_{air} , Estp_{air} \right) \cdot Cstd_{air} \quad (40)$$

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365} \quad (41)$$

Explanation of symbols

$Elocal_{air}$	local direct emission rate to air during episode	[kg · d^{-1}]	eq. (5)
$Estp_{air}$	local indirect emission to air from STP during episode	[kg · d^{-1}]	eq. (35)
$Cstd_{air}$	concentration in air at source strength of 1 kg · d^{-1}	[mg · m^{-3}]	2.78.10^{-4}
Temission	number of days per year that the emission takes place	[d · year^{-1}]	App. IB
$Clocal_{air}$	local concentration in air during emission episode	[mg · m^{-3}]	
$Clocal_{air,ann}$	annual average concentration in air, 100 m from point source	[mg · m^{-3}]	

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air} \quad (42)$$

Explanation of symbols

$Clocal_{air,ann}$	annual average local concentration in air	[mg · m^{-3}]	eq. (40)
$PECregional_{air}$	regional concentration in air	[mg · m^{-3}]	2.3.8.7
$PEClocal_{air,ann}$	annual average predicted environmental conc. in air	[mg · m^{-3}]	

The calculation of deposition flux is slightly more complex because of the dependence of the deposition flux on the fraction of the substance that is associated with the aerosols. In calculating the deposition flux, the emissions from the two sources (direct and STP) are summed:

$$DEPtotal = \left(Elocal_{air} + Estp_{air} \right) \cdot \left(Fass_{aer} \cdot DEPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right) \quad (43)$$

$$DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365} \quad (44)$$

Explanation of symbols

$Elocal_{air}$	local direct emission rate to air during emission episode	[kg · d^{-1}]	eq. (5)
$Estp_{air}$	local indirect emission to air from STP during episode	[kg · d^{-1}]	eq. (35)
$Fass_{aer}$	fraction of the substance bound to aerosol	[-]	eq. (19)
$DEPstd_{aer}$	standard deposition flux of aerosol-bound compounds at a source strength of 1 kg · d^{-1}	[mg · m^{-2} · d^{-1}]	1 · 10^{-2}
$DEPstd_{gas}$	deposition flux of gaseous compounds as a function of Henry's Law constant, at a source strength of 1 kg · d^{-1}	[mg · m^{-2} · d^{-1}]	
	^{10}logHENRY ≤ -2:		5 · 10^{-4}
	-2 < ^{10}logHENRY ≤ 2:		4 · 10^{-4}
	^{10}logHENRY > 2:		3 · 10^{-4}
Temission	number of days per year that the emission takes place	[d · yr^{-1}]	App. IB
DEPtotal	total deposition flux during emission episode	[mg · m^{-2}.d^{-1}]	
$DEPtotal_{ann}$	annual average total deposition flux	[mg.m^{-2}.d^{-1}]	

2.3.8.3 Calculation of PEClocal for the aquatic compartment

In this section, the following parameters are derived:

- local concentration in surface water during emission episode;
- annual average local concentration in surface water.

The effluent of the sewage treatment plant is diluted into the surface water. **Figure 9** shows the most important fate processes of the aquatic compartment. For the calculations, the following assumptions are made:

- complete mixing of the effluent in surface water is assumed as a representative exposure situation for the aquatic eco-system;
- for the first approach in the local assessments, volatilisation, degradation, and sedimentation are ignored because of the short distance between the point of effluent discharge and the exposure location.

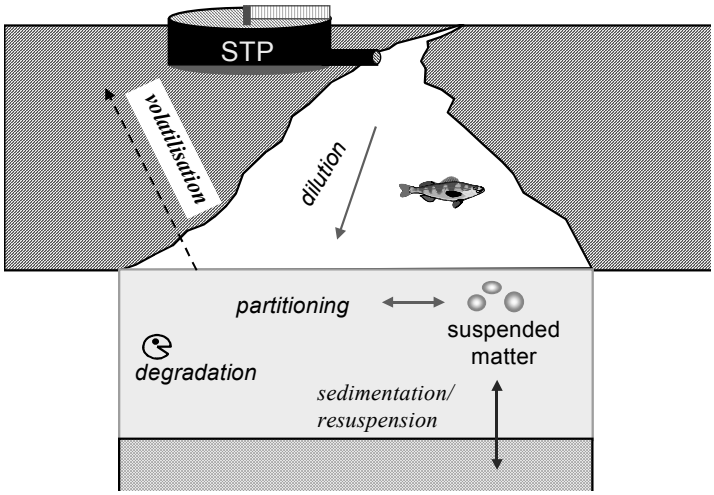

Figure 9 ***Fate processes in surface water***

The calculation of the PEClocal for the aquatic compartment involves several sequential steps (see also **Figure 9**). It includes the calculation of the discharge concentration of a STP to a water body, dilution effects and removal from the aqueous medium by adsorption to suspended matter.

Dilution in the receiving surface water and adsorption to suspended matter

The distance from the point of discharge where complete mixing may be assumed will vary between different locations. A fixed dilution factor may be applied. Dilution factors are dependent on flow rates and the industry specific discharge flow. Due to the different seasonal, climatic and geographical conditions in the Member States, those dilution factors may vary over wide ranges. They have been reported in a range from 1 (e.g. dry riverbeds in summer) up to 100,000 (de Greef and de Nijs, 1990). The dilution factor is generally linked to the release scenario of the use category. For example, for consumer products an average dilution factor for sewage from municipal treatment plants of 10 is recommended. This is also regarded as a default dilution value for other types of substances if no specific data are available.

When a substance is released to surface water predominately as particles (e.g. as precipitates or incorporated in small material pieces – see Section 2.3.3.5) this may lead to overestimation of $PEC_{surface\ water}$ and underestimation of $PEC_{sediment}$. If this is expected to occur it should be considered in the further evaluation (e.g. when comparing PEC with monitoring data and in the risk characterisation).

In certain circumstances, it may be possible to identify specific emission points which would allow the use of more precise information regarding the available distribution and fate processes.

Such site-specific assessments should only be used when it is known that all the emissions emanating from the particular point in the life-cycle e.g. manufacture, arise from a limited number of specific and identifiable sites. In these circumstances each specific point of release will need to be assessed individually. If it is not possible to make this judgement, then the default assumptions should be applied. In site-specific assessments, due account can be taken of the true dilution available to the given emission as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC. Normally, only dilution and adsorption to suspended sediment need to be considered but site-specific conditions may indicate that local distribution models can be used.

It must be noted that with the assumption of complete mixing of the effluent in the surface water no account is taken of the fact that in reality in the mixing zone higher concentrations will occur. For situations with relatively low dilution factors this mixing-zone effect can be accepted. For situations with very high dilution factors, however, the mixing zones may be very long and the overall area that is impacted by the effluent before it is completely mixed can be very substantial. Therefore, in case of site-specific assessments the dilution factor that is applied for calculation of the local concentration in surface water should not be greater than 1000.

If no measured data are available on the partition coefficient between suspended matter and water, Kp_{susp}, it can be estimated from the Koc of the substance, determined for other sorbents like soil or sediments (Section 2.3.5) by taking into account different organic carbon contents of the media.

For some substances it may be possible that PECs are calculated in water which are in excess of the water solubility. These results need to be interpreted carefully on a case-by-case basis. The concentration in surface water will not be corrected, but the result needs to be flagged. The PEC has to be interpreted based on the effects found in the aquatic toxicity tests.

In a situation where a substance is released through several point sources into the same river, the resulting cumulative concentration may in a first approach be estimated by assuming it to be released from one point source. If this PEC leads to "concern" then refined approaches may be used, such as river flow models, e.g. OECD (1992a) which address the specific emission pattern as well as river parameters.

The local concentration in surface water is calculated as follows.

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION} \qquad (45)$$

Explanation of symbols

$Clocal_{eff}$	concentration of the substance in the STP effluent	$[mg \cdot l^{-1}]$	eq. (33)
Kp_{susp}	solids-water partitioning coefficient of suspended matter	$[l \cdot kg^{-1}]$	eq. (23)
$SUSP_{water}$	concentration of suspended matter in the river	$[mg \cdot l^{-1}]$	15
DILUTION	dilution factor	[-]	10
$Clocal_{water}$	local concentration in surface water during emission episode	$[mg \cdot l^{-1}]$	

When considering the available dilution, account should be taken of the fluctuating flow-rates of typical receiving waters. The low-flow rate (or 10^{th} percentile) should always be used. Where only average flows are available, the flow for dilution purposes should be estimated as one third of this average. When a site-specific assessment is appropriate, the actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate (this approach should only be used for rivers, not for estuaries or lakes):

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}} \tag{46}$$

Explanation of symbols

$EFFLUENT_{stp}$	effluent discharge rate of stp	$[l \cdot d^{-1}]$	eq. (34)
FLOW	flow rate of the river	$[l \cdot d^{-1}]$	data set
DILUTION	dilution factor at the point of complete mixing	[-]	(max. = 1000)

For indirect human exposure and secondary poisoning, an annual average concentration in surface water is calculated:

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365} \tag{47}$$

Explanation of symbols

$Clocal_{water}$	local concentration in surface water during emission episode	$[mg \cdot l^{-1}]$	eq. (45)
Temission	number of days per year that the emission takes place	$[d \cdot yr^{-1}]$	App. IB
$Clocal_{water,ann}$	annual average local concentration in surface water	$[mg \cdot l^{-1}]$	

The concentration at the regional scale ($PECregional_{water}$) is used as background concentration for the local scale. Therefore, these concentrations are summed:

$$PEClocal_{water} = Clocal_{water} + PECregional_{water} \tag{48}$$

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECregional_{water} \tag{49}$$

Explanation of symbols

$Clocal_{water}$	local concentration in surface water during episode	$[mg \cdot l^{-1}]$	eq. (45)
$Clocal_{water,ann}$	annual average concentration in surface water	$[mg \cdot l^{-1}]$	eq. (47)
$PECregional_{water}$	regional concentration in surface water	$[mg \cdot l^{-1}]$	2.3.8.7
$PEClocal_{water}$	predicted environmental concentration during episode	$[mg \cdot l^{-1}]$	
$PEClocal_{water,ann}$	annual average predicted environmental concentration	$[mg \cdot l^{-1}]$	

2.3.8.4 Calculation of PEClocal for sediment

In this section, the following parameter is derived:

- local concentration in sediment during the emission episode.

PEClocal for sediment can be compared to the PNEC for sediment dwelling organisms. The concentration in freshly deposited sediment is taken as the PEC for sediment, therefore, the properties of suspended matter are used. The concentration in bulk sediment can be derived from the corresponding water body concentration, assuming a thermodynamic partitioning equilibrium (see also Di Toro et al., 1991):

$$PEClocal_{sed} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water} \cdot 1000 \qquad (50)$$

Explanation of symbols

$PEClocal_{water}$	concentration in surface water during emission episode	[mg.l^{-1}]	eq. (48)
$K_{susp\text{-}water}$	suspended matter-water partitioning coefficient	[m^3.m^{-3}]	eq. (24)
RHO_{susp}	bulk density of suspended matter	[kg.m^{-3}]	eq. (18)
$PEClocal_{sed}$	predicted environmental concentration in sediment	[mg.kg^{-1}]	

Highly adsorptive substances may not be considered adequately with the approach described above, as they are often not in equilibrium distribution between water and suspended matter because of their cohesion to the suspended matter; however they may be desorbed after ingestion by benthic or soil organisms.

In the case when release to the surface water predominately occurs as particles (see Section 2.3.8.3) this calculation may underestimate the sediment concentration. If this is expected to occur it should be considered in the further evaluation (e.g. when comparing PEC with monitoring data and in the risk characterisation).

2.3.8.5 Calculation of PEClocal for the soil compartment

In this section, the following parameters are derived:

- local concentration in agricultural soil (averaged over a certain time period);
- local concentration in grassland (averaged over a certain time period);
- percentage of steady-state situation (to indicate persistency).

Exposure assessment for the soil compartment is important with respect to exposure of terrestrial organisms. Furthermore, crops are grown on agricultural soils for human consumption, and cattle, producing meat and milk, are grazing on grasslands. **Figure 10** shows the most important fate processes in the soil compartment.

Guidance for calculating PEClocal in soil is given for the following exposure routes:

- application of sewage sludge in agriculture;
- dry and wet deposition from the atmosphere.

Direct application of substances (on the basis of the maximum recommended application rate; e.g. pesticide adjuvants or fertilisers) is not taken into account. Guidance may need to be developed in the future.

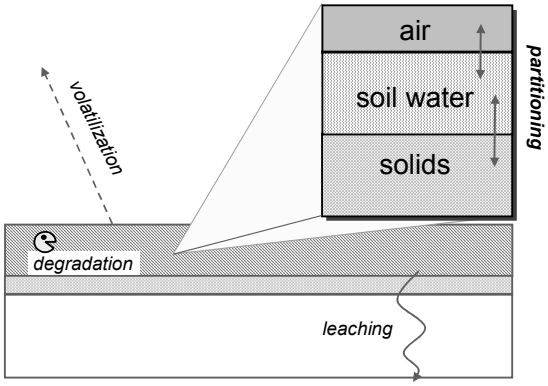

Figure 10 Fate processes in the soil compartment.

For sludge application to agricultural soil an application rate of 5,000 kg/ha dry weight per year is assumed while for grassland a rate of 1000 kg/ha/yr should be used. Sludge application is treated as a single event once a year. The contribution to the overall impact from wet and dry deposition is based on the emission calculation of a point source (Section 2.3.8.2) and is related to a surrounding area within 1000 m from that source. The deposition is averaged over the whole area.

Atmospheric deposition is assumed to be a continuous flux throughout the year. It should be noted that the deposition flux is averaged over a year. This is obviously not fully realistic, since the deposition flux is linked to the emission episode. Averaging is done to facilitate calculation of a steady-state level. Furthermore, it is impossible to indicate when the emission episode takes place within a year: in the beginning of the growing season, any impact on exposure levels will be large, after the growing season, the impact may well be insignificant. Therefore, averaging represents an appropriate scenario choice.

The PEC in agricultural soil is used for two purposes:

- for risk characterisation of terrestrial ecosystems (Section 4);
- as a starting point for the calculation of indirect human exposure via crops and cattle products (see Chapter 2: Risk Assessment for Human Health).

There are several extensive numerical soil and groundwater models available (mainly for pesticides). These models, however, require a detailed definition of soil and environmental characteristics. This makes this type of models less appropriate for a generic risk assessment at EU-level. For the initial assessment, a simplified model is used. The top layer of the soil compartment is described as one compartment, with an average influx through aerial deposition and sludge application, and a removal from the box by degradation, volatilisation, leaching, and other processes if relevant. The concentration in this soil box can now be described with a simple differential equation.

The initial concentration, $C_{soil}(0)$, is governed by the input of the substance through sludge application.

$$\frac{dC_{soil}}{dt} = - k \cdot C_{soil} + D_{air} \qquad (51)$$

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	eq. (52)
t	time	[d]	
k	first order rate constant for removal from top soil	[d^{-1}]	eq. (56)
C_{soil}	concentration in soil	[mg · kg^{-1}]	

In the formula above, the aerial deposition flux is used in mg substance per kg of soil per day. D_{air} can be derived by converting the total deposition flux ($DEPtotal_{ann}$) as follows:

$$D_{air} = \frac{DEPtotal_{ann}}{DEPTH_{soil} \cdot RHO_{soil}} \tag{52}$$

Explanation of symbols

$DEPtotal_{ann}$	annual average total deposition flux	[mg · m^{-2} · d^{-1}]	eq. (44)
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 11
RHO_{soil}	bulk density of soil	[kg · m^{-3}]	eq. (18)
D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	

The differential equation (51) has an analytical solution, given by:

$$C_{soil}(t) = \frac{D_{air}}{k} - \left[\frac{D_{air}}{k} - C_{soil}(0) \right] \cdot e^{-k\,t} \tag{53}$$

With this equation, the concentration can be calculated at each moment in time, when the initial concentration in that year is known.

Accumulation of the substance may occur when sludge is applied over consecutive years. This is illustrated in **Figure 11**. As a realistic worst-case exposure scenario, it is assumed that sludge is applied for 10 consecutive years. To indicate for potential persistency of the substance, the percentage of the steady-state situation is calculated. As shown in **Figure 11**, the concentration in soil is not constant in time.

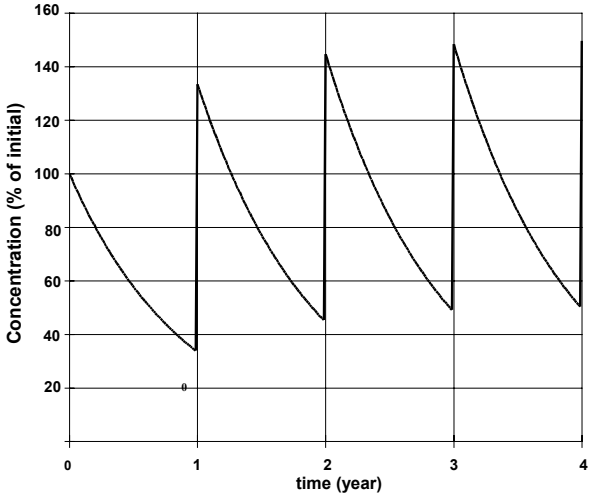

Figure 11 Accumulation in soil due to several years of sludge application

The concentration will be high just after sludge application (in the beginning of the growth season), and lower at the end of the year due to removal processes. Therefore, for exposure of the endpoints, the concentration needs to be averaged over a certain time period. Different averaging times should be considered for these endpoints: for the ecosystem a period of 30 days after application of sludge is used. In

order to determine biomagnification effects and indirect human exposure, it is more appropriate to use an extended period of 180 days.

This averaging procedure is illustrated in **Figure 12** where the average concentration is given by the area of the shaded surface, divided by the number of days.

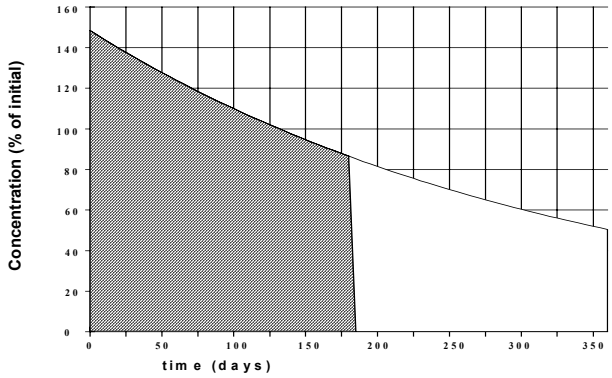

Figure 12 The concentration in soil after 10 years. The shaded area is the integrated concentration over a period of 180 days

The local concentration in soil is defined as the average concentration over a certain time period T. The average concentration over T days is given by:

$$Clocal_{soil} = \frac{1}{T} \cdot \int_0^T C_{soil}\ (t)\ dt \qquad (54)$$

Solving this equation for the range 0 to T gives the final equation for the average concentration in this period:

$$Clocal_{soil} = \frac{D_{air}}{k} + \frac{1}{k\,T}\left[\ C_{soil}\,(0) - \frac{D_{air}}{k}\ \right] \cdot \left[1 - e^{-kT}\right] \qquad (55)$$

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	eq. (52)
T	averaging time	[d]	Table 11
k	first order rate constant for removal from top soil	[d^{-1}]	eq. (56)
C_{soil} (0)	initial concentration (after sludge application)	[mg · kg^{-1}]	eq. (63)
$Clocal_{soil}$	average concentration in soil over T days	[mg · kg^{-1}]	

Derivation of the removal rate constants

The total rate constant for removal is made up of several parts:

- biodegradation rate constant;
- volatilisation of substance from soil;
- leaching to deeper soil layers.

Other removal processes may be important in some cases (e.g. uptake by plants). If rate constants are known for these processes, they may be added to the total removal. The overall removal rate constant is given by:

$$k = k_{volat} + k_{leach} + kbio_{soil} \qquad (56)$$

Explanation of symbols

k_{volat}	pseudo-first order rate constant for volatilisation from soil	[d^{-1}]	eq. (57)
k_{leach}	pseudo-first order rate constant for leaching from top soil	[d^{-1}]	eq. (58)
$kbio_{soil}$	pseudo-first order rate constant for biodegradation in soil	[d^{-1}]	Table 8
k	first order rate constant for removal from top soil	[d^{-1}]	

The diffusive transfer from soil to air is estimated using the classical two-film resistance model. The soil-side of the interface is treated as a pair of parallel resistances (air phase and water phase of soil) (Mackay et al., 1992). The rate constant for volatilisation from soil is given by:

$$\frac{1}{k_{volat}} = \left(\frac{1}{kasl_{air} \cdot K_{air\text{-}water}} + \frac{1}{kasl_{soilair} \cdot K_{air\text{-}water} + kasl_{soilwater}} \right) \cdot K_{soil\text{-}water} \cdot DEPTH_{soil} \qquad (57)$$

Explanation of symbols

$kasl_{air}$	partial mass transfer coeff. at air-side of the air-soil interface	[$m \cdot d^{-1}$]	120
$kasl_{soilair}$	partial mass transfer coeff. at soilair-side of the air-soil int.	[$m \cdot d^{-1}$]	0.48
$kasl_{soilwater}$	partial mass transfer coeff. at soilwater-side of the air-soil int.	[$m \cdot d^{-1}$]	$4.8 \cdot 10^{-5}$
$K_{air\text{-}water}$	air-water equilibrium distribution constant	[$m^3 \cdot m^{-3}$]	eq. (22)
$K_{soil\text{-}water}$	soil-water partitioning coefficient	[$m^3 \cdot m^{-3}$]	eq. (24)
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 11
k_{volat}	pseudo first-order rate constant for volatilisation from soil	[d^{-1}]	

A pseudo first-order rate constant for leaching can be calculated from the amount of rain flushing the liquid-phase of the soil compartment:

$$k_{leach} = \frac{Finf_{soil} \cdot RAINrate}{K_{soil\text{-}water} \cdot DEPTH_{soil}} \qquad (58)$$

Explanation of symbols

$Finf_{soil}$	fraction of rain water that infiltrates into soil	[-]	0.25
RAINrate	rate of wet precipitation (700 mm/year)	$[m.d^{-1}]$	$1.92 \cdot 10^{-3}$
$K_{soil\text{-}water}$	soil-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	eq. (24)
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 11
k_{leach}	pseudo first-order rate constant for leaching from soil layer	$[d^{-1}]$	

Derivation of the initial concentration after 10 years of sludge application

As a realistic worst-case assumption for exposure, it is assumed that sludge application takes place for 10 consecutive years. To be able to calculate the concentration in this year averaged over the time period T (equation (55)), an initial concentration in this year needs to be derived. For this purpose, the contributions of deposition and sludge applications are considered separately.

The concentration due to 10 years of continuous deposition only, is given by applying equation (53) with an initial concentration of zero and 10 years of input:

$$Cdep_{soil\,10}(0) = \frac{D_{air}}{k} - \frac{D_{air}}{k} \cdot e^{-365 \cdot 10 \cdot k} \tag{59}$$

For sludge application, the situation is more complicated as this is not a continuous process. The concentration just after the first year of sludge application is given by:

$$Csludge_{soil\,1}(0) = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO_{soil}} \tag{60}$$

Explanation of symbols

C_{sludge}	concentration in dry sewage sludge	$[mg \cdot kg^{-1}]$	eq. (36)
$APPL_{sludge}$	dry sludge application rate	$[kg \cdot m^{-2} \cdot yr^{-1}]$	Table 11
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 11
RHO_{soil}	bulk density of soil	$[kg \cdot m^{-3}]$	eq. (18)
$Csludge_{soil\,1}(0)$	concentration in soil due to sludge in first year at t=0	$[mg \cdot kg^{-1}]$	

The fraction of the substance that remains in the top soil layer at the end of a year is given by:

$$Facc = e^{-365\,k} \tag{61}$$

Explanation of symbols

k	first order rate constant for removal from top soil	$[d^{-1}]$	eq. (56)
Facc	fraction accumulation in one year	[-]	

At the end of each year, a fraction Facc of the initial concentration remains in the top-soil layer. The initial concentration after 10 applications of sludge is given by:

$$Csludge_{soil\,10}\ (0)\ =\ Csludge_{soil\,1}\ (0)\ \cdot\ \left[\ 1\ +\ \sum_{n=1}^{9}\ Facc^{n}\ \right] \qquad (62)$$

The sum of both the concentration due to deposition and sludge is the initial concentration in year 10:

$$C_{soil\,10}\ (0)\ =\ Cdep_{soil\,10}\ (0)\ +\ Csludge_{soil\,10}\ (0) \qquad (63)$$

This initial concentration can be used in equation (54) to calculate the average concentration in soil over a certain time period.

Indicating persistency of the substance in soil

Ten consecutive years of accumulation may not be sufficient for some substances to reach a steady-state situation. These substances may accumulate for hundreds of years. To indicate potential problems of persistency in soil, the fraction of the steady-state concentration can be derived:

$$Fst\text{-}st\ =\ \frac{C_{soil\,10}\ (0)}{C_{soil\,\infty}\ (0)} \qquad (64)$$

Explanation of symbols

C_{soil} 10 (0)	initial concentration after 10 years	[mg · kg^{-1}]	eq. (63)
$C_{soil\,\infty}$ (0)	initial concentration in steady-state situation	[mg · kg^{-1}]	eq. (65)
Fst-st	fraction of steady-state in soil achieved	[-]	

The initial concentration in the steady-state year is given by:

$$C_{soil\,\infty}\ (0)\ =\ \frac{D_{air}}{k}\ +\ Csludge_{soil\,1}\ (0)\ \cdot\ \frac{1}{1\ -\ Facc} \qquad (65)$$

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	eq. (52)
k	first order rate constant for removal from top soil	[d^{-1}]	eq. (56)
Facc	fraction accumulation in one year	[-]	eq. (61)
$Csludge_{soil\,1}$ (0)	concentration in soil due to sludge in first year at t=0	[mg · kg^{-1}]	eq. (60)
$C_{soil\infty}$(0)	initial concentration in steady-state situation	[mg · kg^{-1}]	

Calculation of $PEClocal_{soil}$

For soil, three different PECs are calculated, for different endpoints (**Table 11**).

Table 11 Characteristics of soil and soil-use for the three different endpoints

	Depth of soil compartment [m]	Averaging time [days]	Rate of sludge application [$kg_{dwt} \cdot m^{-2} \cdot year^{-1}$]	Endpoint
$PEClocal_{soil}$	0.20	30	0.5	terrestrial ecosystem
$PEClocal_{agr.\ soil}$	0.20	180	0.5	crops for human consumption
$PEClocal_{grassland}$	0.10	180	0.1	grass for cattle

The "depth of soil" represents the depth range for the top soil layer which is of interest. The depth of 20 cm is taken because this range usually has a high root density of crops, and represents the ploughing depth. For grassland, the depth is less since grasslands are not ploughed. The averaging period of 180 days for crops is chosen as a representative growing period for crops. For grassland this period represents a reasonable assumption for the period that cattle is grazing on the field. For the ecosystem a period of 30 days is taken as a relevant time period with respect to chronic exposure of soil organisms.

The concentration at the regional scale is used as background concentration for the local scale. For this purpose, the concentration in unpolluted soil needs to be applied ("natural soil", only input through deposition). Otherwise, sludge application is taken into account twice.

$$PEClocal_{soil} = Clocal_{soil} + PECregional_{natural\ soil} \quad (66)$$

Explanation of symbols

$Clocal_{soil}$	local concentration in soil	$[mg \cdot kg^{-1}]$	eq. (54)
$PECregional_{natural\ soil}$	regional concentration in natural soil	$[mg \cdot kg^{-1}]$	2.3.8.7
$PEClocal_{soil}$	predicted environmental conc. in soil	$[mg \cdot kg^{-1}]$	

The equation for deriving the concentration in the pore water is:

$$PEClocal_{soil,\ porew} = \frac{PEClocal_{soil} \cdot RHO_{soil}}{K_{soil\text{-}water} \cdot 1000} \quad (67)$$

Explanation of symbols

$PEClocal_{soil}$	predicted environmental conc. in soil	$[mg \cdot kg^{-1}]$	eq. (66)
$K_{soil\text{-}water}$	soil-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	eq. (24)
RHO_{soil}	bulk density of wet soil	$[kg \cdot m^{-3}]$	eq. (18)
$PEClocal_{soil,porew}$	predicted environmental conc. in porewater	$[mg \cdot l^{-1}]$	

2.3.8.6 Calculation of concentration in groundwater

In this section, the following parameter is derived:

- local concentration in groundwater.

The concentration in groundwater is calculated for indirect exposure of humans through drinking water. For the calculation of groundwater levels, several numerical models are available (mainly for pesticides). These models, however, require a characterisation of the soil on a high level of detail. This makes these models less appropriate for the initial standard assessment. Therefore, as an indication for potential groundwater levels, the concentration in porewater of agricultural soil is taken. It should be noted that this is a worst-case assumption, neglecting transformation and dilution in deeper soil layers.

$$PEClocal_{grw} = PEClocal_{agr.soil,porew} \quad (68)$$

Explanation of symbols

$PEClocal_{agr.soil,porew}$	predicted environmental conc. in porewater	$[mg \cdot l^{-1}]$	eq. (67)
$PEClocal_{grw}$	predicted environmental conc. in groundwater	$[mg \cdot l^{-1}]$	

2.3.8.7 Calculation of PECregional

In this section, the following parameters are derived:

- Regional exposure concentrations in all environmental compartments.

Regional computations are done by means of multimedia fate models based on the fugacity concept. Recently, models have been described by Mackay et al. (1992), Van de Meent (1993) and Brandes et al., 1996) (SimpleBox). These models are box models, consisting of a number of compartments (see **Figure 13**) which are considered homogeneous and well mixed. A substance released into the model scenario is distributed between the compartments according to the properties of both the substance and the model environment. Several types of fate processes are distinguished in the regional assessment, as drawn in **Figure 13**:

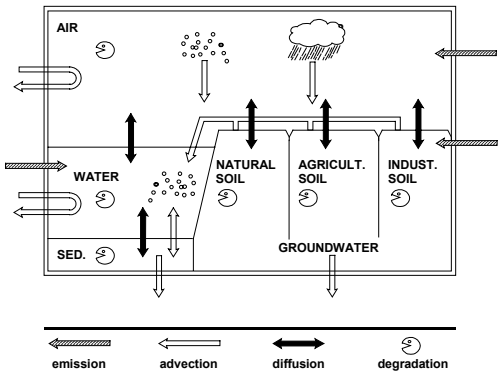

Figure 13 The relevant emission and distribution routes

- emission, direct and indirect (via STP) to the compartments air, water, industrial soil, and agricultural soil;
- degradation, biotic and abiotic degradation processes in all compartments;

- diffusive transport, as e.g. gas absorption and volatilisation. Diffusive mass transfer between two compartments goes both ways, the net flow may be either way, depending on the concentration in both compartments;
- advective transport, as e.g. deposition, run-off, erosion. In the case of advective transport, a substance is carried from one compartment into another by a carrier that physically flows from one compartment into the other. Therefore, advective transport is strictly one-way.

Substance input to the model is regarded as continuous and equivalent to continuous diffuse emission. The results from the model are steady-state concentrations, which can be regarded as estimates of long-term average exposure levels. The fact that a steady state between the compartments is calculated, does not imply that the compartment to which the emission takes place is of no importance.

In a Mackay-type level III model, the distribution and absolute concentrations may highly depend upon the compartment of entry.

Advective import and export (defined as inflow from outside the model or outflow from the model environment) can be very important for the outcome of both regional and local model calculations. Therefore, the concentration of a substance at the "border" of the region must be taken into account. This is defined as the background concentration of a substance. The background concentration in a local model can be obtained from the outcome of the regional model. For substances with many relatively small point sources, this background concentration may represent a significant addition to the concentration from a local source. The background concentration in the regional model has to be calculated using a similar box model of a larger scale, e.g. with the size of the European continent. In this continental model, however, it is assumed that no inflow of air and water across the boundaries occurs. Furthermore it is assumed that all substance releases enter into this continental environment. The resulting steady-state concentrations are then used as transboundary or background concentrations in the regional model. The continental and regional computations should thus be done in sequence. **Figure 1** visualises the relationship between the concentrations calculated for the different model scales. For both the regional and continental scale, the total emission amounts (through diffuse and point sources, summed over all stages of the life-cycle) are used.

For the PECregional calculation, in contrast to PEClocal, an average percentage connection rate to STPs should be included in the calculation. This leads to a more realistic estimation of the likely background concentration on a regional scale. For the purposes of the generic regional model, a STP connection rate of 80% (the EU average according to Appendix XII) will be assumed.

The results from the regional model should be interpreted with caution. The environmental concentrations are averages for the entire regional compartments (which were assumed well mixed). Locally, concentrations may be much higher than these average values. Furthermore, there is a considerable degree of uncertainty due to the uncertainty in the determination of input parameters (e.g. degradation rates, partitioning coefficients).

Model parameters for PECregional

When calculating the PECregional it is important which modelling parameters are chosen and what fraction of the total emissions is used as emission for the region. There are two different possibilities:

- calculation of a PECregional on the basis of a standardised regional environment with agreed model parameters;
- calculation of a PECregional on the basis of country specific model parameters.

A standardised regional environment should be used for the first approach in the calculation of PECregional. When more specific information is available on the location of production /emission sites, this information can be applied to refine the regional assessment. The second approach may sometimes result in a better estimation of the concentrations for a specific country. However, depending on the information on production site location, it will lead to a number of different PEC values which makes a risk characterisation at EU level more complicated.

Calculations are performed for a densely populated area of 200·200 km with 20 million inhabitants. Unless specific information on use or emission per capita is available, it is assumed that 10% of the European production and use takes place within this area, i.e. 10% of the estimated emission is used as input for the region. The model parameters proposed for this standard region are given in **Table 12**. It should be noted that it is extremely difficult to select typical or representative values for a standard European region. Therefore, the rationale behind the values of **Table 12** is limited. Nevertheless, these values present a starting point for the regional scale assessments. Characterisation of the environmental compartments for the regional model should be done according to the values in **Table 5**.

Table 12 Proposed model parameters for regional model

Parameter	Value in regional model
area of the regional system	4.104 km^2
area fraction of water	0.03
area fraction of natural soil	0.60
area fraction of agricultural soil	0.27
area fraction of industrial/urban soil	0.10
mixing depth of natural soil	0.05 m
mixing depth of agricultural soil	0.2 m
mixing depth of industrial/urban soil	0.05 m
atmospheric mixing height	1000 m
depth of water	3 m
depth of sediment	0.03 m
fraction of the sediment compartment that is aerobic	0.10
average annual precipitation	700 mm·yr-1
wind speed	3 m·s-1
residence time of air	0.7 d
residence time of water	40 d
fraction of rain water infiltrating soil	0.25
fraction of rain water running off soil	0.25
EU average connection percentage to STP	80%

The area fractions for water and for natural, agricultural and industrial/urban soils, are average values obtained from ECETOC (1994b), supplemented with data received from Sweden and Finland. Data for Norway and Austria are obtained from the FAO statistical databases (http://apps.fao.org/). The residence time for air (defined as the time between air entering and leaving the region) of 0.7 days is derived from the wind speed of 3 m/s and the area of the region. The residence time of water of 40 days is selected as a reasonable average for the European situation.

The amount of wastewater discharged, is the product of the amount of wastewater discharged per person equivalent and the number of inhabitants of the system. Using a flow per capita of 200 $l \cdot d^{-1}$ (equivalent to the value used in the SimpleTreat model, see **Table 9**) and a population of 20 million, this results in an additional water flow through the model environment of $4.0 \cdot 10^6$ $m^3 \cdot d^{-1}$. The inflow caused by inflowing riverwater, is $6.5 \cdot 10^7$ $m^3 \cdot d^{-1}$.

In addition to the environmental characteristics of the region, selected intermedia mass transfer coefficients are required in the multimedia fugacity model to ensure comparability of the outcome with other models. These transfer coefficients are summarised in **Table 13**.

Table 13 Intermedia mass transfer coefficients

Parameter	Value
air-water interface: air side partial mass transfer coefficient	$1.39 \cdot 10^{-3}$ $m \cdot s^{-1}$
air-water interface: water side partial mass transfer coefficient	$1.39 \cdot 10^{-5}$ $m \cdot s^{-1}$
Aerosol deposition rate	0.001 $m \cdot s^{-1}$
air-soil interface: air side partial mass transfer coefficient	$1.39 \cdot 10^{-3}$ $m \cdot s^{-1}$
air-soil interface: soilair side partial mass transfer coefficient	$5.56 \cdot 10^{-6}$ $m \cdot s^{-1}$
air-soil interface: soilwater side partial mass transfer coefficient	$5.56 \cdot 10^{-10}$ $m \cdot s^{-1}$
sediment-water interface: water side partial mass transfer coefficient	$2.78 \cdot 10^{-6}$ $m \cdot s^{-1}$
sediment-water interface: pore water side partial mass transfer coefficient	$2.78 \cdot 10^{-8}$ $m \cdot s^{-1}$
net sedimentation rate	3 $mm \cdot yr^{-1}$

Model parameters for the continental concentration

The continental box covers all 15 EU countries and Norway and similar percentages for water and natural, agricultural and industrial/urban soils as given in **Table 14**. All other parameters are similar to the ones given in the preceding tables. Emission estimation to this continental box should be based on the EU-wide production volume of the substance. The resulting concentrations in water and air must be used as background concentrations (i.e. concentrations in water or air that enter the system) in the regional model. When the model is built according to **Figure 1** it is assumed that no inflow of the substance into the continental system takes place. More recent versions of multimedia models do also contain so-called global scales for different temperature regions, for instance moderate, tropic and arctic (see e.g. Brandes et al., 1996). In this case the continent is embedded in the moderate scale just like the region is embedded in the continent. The size of the total global scale is that of the northern hemisphere. The global scales allow for a more accurate estimation of continental concentrations

although this effect tends to be marginal. However, the global scales provide more insight in the ultimate persistence of the chemical.

Table 14 Parameters for continental model

Parameter	Value in continental model
area of the continental system	$3.56 \cdot 10^6$ km^2
area fraction of water	0.03
area fraction of natural soil	0.60
area fraction of agricultural soil	0.27
area fraction of industrial/urban soil	0.10

2.4 SUMMARY OF PECs DERIVED

In summary, the local estimations yield the following input and output information:

Input

Physico-chemical properties	Section 2.3.2
Characterisation of the environment	Table 5
Emission data	Section 2.3.3.3
Partitioning coefficients	Section 2.3.5
Degradation rates	Section 2.3.6
Fate in sewage treatment plants	Section 2.3.7

Output

$PEC_{microorganisms}$	local PEC for microorganisms in the STP	[mg · l^{-1}]	eq. (38), (36)
$PEClocal_{water}$	local PEC in surface water (dissolved) during episode	[mg · l^{-1}]	eq. (48)
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	[mg · l^{-1}]	eq. (49)
$PEClocal_{sed}$	local PEC in sediment (total)	[mg · kg^{-1}]	eq. (50)
$PEClocal_{air,ann}$	annual average local PEC in air (total)	[mg · m^{-3}]	eq. (42)
$PEClocal_{soil}$	local PEC in agricultural soil (total), averaged over 30 days	[mg · kg^{-1}]	eq. (66)
$PEClocal_{agr.soil}$	local PEC in agricultural soil (total), averaged over 180 days	[mg · kg^{-1}]	eq. (66)
$PEClocal_{grassland}$	local PEC in grassland (total), averaged over 180 days	[mg · kg^{-1}]	eq. (66)
$PEClocal_{agr.soil,porew}$	local PEC in porewater of agricultural soil	[mg · l^{-1}]	eq. (67)
$PEClocal_{grassland,porew}$	local PEC in porewater of grassland	[mg · l^{-1}]	eq. (67)
$PEClocal_{grw}$	local PEC in groundwater under agricultural soil	[mg · l^{-1}]	eq. (68)

The regional estimations yield the following input and output information:

Input

Physico-chemical properties	Section 2.3.2
Characterisation of the environment	Table 4
Parameters of the regional compartments	Table 11, Table 12, Table 13
Emission data	Section 2.3.3.3
Partitioning coefficients	Section 2.3.5
Degradation rates	Section 2.3.6
Fate in sewage treatment plants	Section 2.3.7

Output

$PECregional_{water}$	regional PEC in surface water (dissolved)	$[mg \cdot l^{-1}]$	Section 2.3.8.7
$PECregional_{air}$	regional PEC in air (total)	$[mg \cdot m^{-3}]$	Section 2.3.8.7
$PECregional_{agr.soil}$	regional PEC in agricultural soil (total)	$[mg \cdot kg^{-1}]$	Section 2.3.8.7
$PECregional_{natural\ soil}$	regional PEC in natural soil (total)	$[mg \cdot kg^{-1}]$	Section 2.3.8.7
$PECregional_{agr.soil,porew}$	regional PEC in porewater of agricultural soils	$[mg \cdot l^{-1}]$	Section 2.3.8.7
$PECregional_{sed}$	regional PEC in sediment (total)	$[mg \cdot kg^{-1}]$	Section 2.3.8.7

2.5 DECISION ON THE ENVIRONMENTAL CONCENTRATION USED FOR RISK CHARACTERISATION

When PECs have been derived from both measured data and calculation, they are compared. If they are not of the same order of magnitude, analysis and critical discussion of divergences are important steps for developing an environmental risk assessment of existing substances. The following cases can be distinguished:

- Calculated PEC ≈ PEC based on measured concentrations

  The result indicates that the most relevant sources of exposure were taken into account. For risk characterisation, the value with the highest confidence should be used;

- Calculated PEC > PEC based on measured concentrations

  This result might indicate that relevant elimination processes were not considered in the PEC calculation or that the employed model was not suitable to simulate the real environmental conditions for the regarded substance. On the other hand measured data may not be reliable or represent only the background concentration or PECregional in the regarded environmental compartment. If the PEC based on measured data has been derived from a sufficient number of representative samples then they should override the model predictions. However if it cannot be demonstrated for the calculated PEC that the scenario is not unrealistically worst-case, the calculated PEC should be preferred.

- Calculated PEC < PEC based on measured concentrations

  This relation between calculated PEC and PEC based on measured concentrations can be caused by the fact that relevant sources of emission were not taken into account when calculating the PEC, or that the used models were not suitable. Similarly, an overestimation of degradation of the compound may be the explanation. Alternative causes may be spillage, a recent change in use pattern or emission reducing measures that are not yet reflected in the samples.

If it is confirmed that the PEC based on measured concentrations is still representative for the exposure situation of the substance further work is needed to elucidate the exposure situation. Other reasons might cause the described divergence:

- there is a transboundary influx;
- a natural source exists;
- the compound represents a metabolite of another substance;
- a retarded remobilisation results from a pool present in other environmental compartments (e.g. from scrap or waste materials or former applications).

If the measured values have passed the procedure of critical statistical and geographical evaluation, a high degree of confidence can be attributed to those data and they shall overwrite the calculated PECs. It is necessary to consider all environmental compartments when the measurements and predictions are made otherwise the possibility of chance agreement may be overlooked.

3 EFFECTS ASSESSMENT

3.1 INTRODUCTION

The effects assessment comprises the following steps of the risk assessment procedure:

- hazard identification: The aim of the hazard identification is to identify the effects of concern. For existing substances and biocidal active substances and substances of concern in biocidal products, the aim is also to review the classification of the substance while for new substances a proposal on classification is done;
- dose (concentration) - response (effect) assessment: At this step the predicted no effect concentration (PNEC), shall, where possible, be determined.

For both steps of the effects assessment it is of high importance to evaluate the data with regard to their adequacy and completeness. The evaluation of adequacy shall address the quality and relevance of data (see Section 3.2). The evaluation of data is of particular importance for existing substances as tests will often be available with non-standard organisms and/or non-standardised methods. It is suitable to start the effects assessment process with the evaluation of the available ecotoxicological data.

As stated in Section 1.2, the environmental compartments considered for the inland environment are the aquatic and terrestrial ecosystem, top predators, microbial activity in a STP, and the atmosphere. This means that for each of these compartments a PNEC has to be derived. A PNEC is regarded as a concentration below which an unacceptable effect will most likely not occur. In principle, the PNEC is calculated by dividing the lowest short-term L(E)C50 or long-term NOEC value by an appropriate assessment factor. The assessment factors reflect the degree of uncertainty in extrapolation from laboratory toxicity test data for a limited number of species to the 'real' environment. Assessment factors applied for long-term tests are smaller as the uncertainty of the extrapolation from laboratory data to the natural environment is reduced. For this reason long-term data are preferred to short-term data.

A detailed assessment of the environmental risk is often only feasible for the water compartment: for new substances the base-set consists of effect data for aquatic organisms only, while for existing substances most of the available data will be for aquatic organisms. For biocides, the core data set comprises effect data on aquatic organisms as well. Therefore, a more detailed description on deriving a $PNEC_{water}$ is described in Section 3.3. For an intermittent release of substances, aquatic organisms may be exposed for only a short period. In these cases, short-term L(E)C50 values are used to derive a $PNEC_{water, intermittent}$. This is described in Section 3.3.2.

The microbial activity in domestic and industrial STPs may be affected. Assessment factors to derive a $PNEC_{microorganisms}$ are given in Section 3.4.

Probably for most compounds no data will be present for sediment-dwelling organisms. Appropriate test systems and standardised guidelines are still under development. The equilibrium partitioning method is proposed as a screening method for derivation of a $PNEC_{sed}$ to compensate for this lack of toxicity data. If sediment test results are available, the $PNEC_{sed}$ is derived from these data by applying assessment factors (see Section 3.5).

Few toxicity data are also available for the soil compartment. Where such data are present, they will normally include only test results from short-term studies. If test data are lacking, the

equilibrium partitioning method can be used to derive a $PNEC_{soil}$. Otherwise, assessment factors are applied (see Section 3.6).

Biotic and abiotic effects, such as acidification, are addressed for the atmosphere. In view of the lack of suitable data and the fact that no adequate methods are available yet to assess both types of effects, a provisional strategy is described in Section 3.7.

Standard assays of ecotoxicological effects usually provide information about the direct toxic effects of a substance. Chemicals showing bioaccumulation and biomagnification may pose an additional threat due to exposure of organisms higher in the food chain, e.g. top predators. This phenomenon is called 'secondary poisoning' and has to be addressed if a chemical fulfils several criteria, e.g. indication of a bioaccumulation potential. If this is the case, the oral intake of a chemical via fish or worms ($PECoral_{fish}$ and $PECoral_{worm}$) is compared to a PNEC for fish- or worm-eating mammals or birds. This approach is described in Section 3.8.

Knowledge on endocrine disrupting effects of some substances is presently under development. When substantial evidence on such effects is available, this should be taken into account on a case-by-case basis in the derivation of the PNEC for each compartment of relevance. Existing knowledge does not allow a more standardised approach for risk assessment of such substances.

It is recognised that experience with several of the described effects assessment methods is lacking. Thus, assessments by use of these types of methods can be uncertain. However, the methods presented make it possible to identify if the compartment under consideration is possibly “of concern” and whether further data, e.g. testing on relevant organisms for that compartment, should be obtained.

The environmental part of the risk assessment should contain some general reflection on the mode of action of the chemical. Cross-reference to relevant sections in the human health part may be important. For example when a chemical is found to have effects on gonad development in fish and similar effects have been observed in laboratory mammals. Identification of similarities in the nature, intensity and time scale of effects between species, as well as in the susceptibilities of different receptors, will allow a better understanding of the actual risk to these organisms to be obtained and help in the identification of issues of concern (IPCS, 2000).

3.2 EVALUATION OF DATA

3.2.1 Ecotoxicity data

During both steps of the effects assessment it is very important to evaluate data with regard to their adequacy and completeness. This is particularly important for existing substances that have been extensively studied where there may be a number of test results available beyond the base-set. This section puts forward general guidelines on the evaluation of ecotoxicity data. The term adequacy is used here to cover the reliability of the available data and the relevance of that data for environmental hazard and risk assessment.

3.2.1.1 Completeness of data

New substances

For new substances data equivalent to those identified in Annex VII A to Directive 67/548 will be available: the base-set. The base-set comprises short- term toxicity data for algae, Daphnia and fish for the aquatic compartment. Data for bacteria (respiration inhibition test) are also part of the base-set. These data are used for assessing the effects on microbial activity in a STP (see Section 3.4). The base-set testing package contains relatively little data that are of relevance to the terrestrial and atmospheric compartments: additional but nevertheless still limited data are obtained at level 1 and 2.

Existing substances

Availability of data for existing substances varies considerably. Regulation 793/93 requires that for priority substances at least the base-set data according to Annex VII A to Directive 67/548 are provided before the risk assessment process begins. However, for many substances more information will be available which can be used in the assessment.

The base-set ensures that short-term effects data are available for fish, Daphnia, algae and bacteria. Within a trophic level, a number of short-term investigations may also be available for several non-standard organisms. In addition, long-term toxicity investigations may be available with several species, standard organisms as well as non-standard organisms. These organisms should be assigned to appropriate trophic levels for the derivation of the PNEC (see Appendix IV and Section 3.3.1). Multi-species tests, investigations with model ecosystems and semi-field tests, are rarely available for substances although in recent years more work has been done in this area (Hill et al., 1994; Knacker and Morgan, 1994).

Active biocidal substances

The data requirements for active biocidal substances are laid down in Annex IIA and Annex IIIA of Directive 98/8. The core data requirements for biocides correspond to the base-set for new substances. However, depending on Product Type and intended use of the biocidal product, additional toxicity data may be required as described in the Technical Notes for Guidance in support of Directive 98/8 on the placing of biocidal products on the market (TNsG on Data Requirements, 2000; http://ecb.jrc.it/biocides/).

3.2.1.2 Adequacy of data

The adequacy of a test data can be defined by two basic elements:

- reliability: covering the inherent quality of a test relating to test methodology and the way that the performance and results of the test are described;
- relevance: covering the extent to which a test is appropriate for a particular hazard or risk assessment.

Only reliable, relevant data can be considered valid for use in the risk assessment.

The assessment of data adequacy therefore involves:

- A review of individual data elements with respect to how the study is conducted and how the results are interpreted; and,
- A critical selection (and rejection) of data in its proper context and in accordance with the purpose of the assessment.

New substances and biocidal substances

The tests for new substances and biocidal substances must be carried out in accordance with the EU testing methods as laid down in Annex V to Directive 67/548[3], or if no EU methods are available or they are not applicable, in accordance with internationally recognised guidelines, preferably those of the OECD (1993b). They must also be conducted in accordance with the principles of good laboratory practice as set out in Council Directive 87/18.

Existing substances

The risk assessment for existing substances starts with the collecting of all available information by the manufacturers, importers, and the rapporteur. Any new tests carried out for risk assessments under Regulation 793/93 should be conducted according to the testing methods laid down in Annex V to Directive 67/548, or if no EU methods are available or they are not applicable, in accordance with internationally recognised guidelines, preferably those of the OECD (1993b). They must also be conducted following good laboratory practice according to Directive 87/18.

This information will probably contain data that have been generated prior to the requirements of GLP being specified and prior to the standardisation of testing methods. However, these data may be used for the risk assessment, if valid conclusions can be drawn from them. This means that the data, and the test methods used to generate them, must be evaluated in order to determine whether they are of sufficient quality for use in risk assessment. Such an evaluation will require the use of expert judgement, but the determination of data as being valid or not valid must be both justified and transparent. The requirements of the standardised test methods and GLP principles should be regarded as a reference when evaluating the available tests. Sufficient information must be available in order to allow a judgement on the reliability of a study to be made.

Greater weight should normally be attached to studies carried out according to current methods (e.g. EU, OECD, or US EPA) (cf. Ahlers et al., 1992; OECD, 1998a). Criteria for data reliability refer to accepted standards:

- a complete test report is available or the test has been described in sufficient detail and the test procedure is in accordance with generally accepted standards. These data are considered valid and can be used for risk assessment;
- the validity of the data cannot be fully established or the test method differs in some respects from the guidelines and the generally accepted scientific standards. Experts must decide in each case whether the test result can be taken into consideration in the risk assessment or is regarded as not valid;

[3] A complete listing of the EC Testing Methods as well as references to the relevant Directives and Official Journals where they can be found are available in the ECB web page <http://ecb.jrc.it/testing-methods>. Some methods can be downloaded from this site as well.

- it is clearly evident that the data are not valid because critical pieces of information are not available and cannot be sourced retrospectively (e.g. it is not possible to establish the identity of the test substance). These data are not considered to be valid for the risk assessment. However, they may be used as an aid in the design of an appropriate test.

In principle, the same criteria apply for tests reported in published literature. The amount of information presented will provide the basis for deciding on the validity of a test result. In general, test results that have been reported in peer reviewed journals are preferred. High quality reviews may be used as supporting information. Summaries or abstract publications may also provide supporting data.

In cases where differing results from similar studies were obtained or an extensive data set is available for an individual species or a taxonomic group, it may be possible to use the distribution of these data to draw general conclusions regarding the toxicity to that species or taxon.

Results from field studies may also be available. These studies can vary widely in the nature of the experimental system: from indoor microcosms to outdoor macrocosms such as experimental streams (Hill et al., 1994). Field studies may provide a better insight into the toxic effects (including indirect effects) of chemicals, as well as factors affecting their routes of exposure (e.g. bioavailability, biodegradation). At present, there are no internationally accepted guidelines for fieldstudies. However, some general guidance has been laid down for the conduction of field studies in aquatic ecosystems (SETAC, 1991; SETAC, 1992; Campbell et al., 1999; Posthuma et al., 2001).

Relevance of data

In order to evaluate the relevance of the available data, it is necessary to judge, *inter alia*, if the appropriate endpoints are studied under relevant conditions and if the substance tested is representative of the substance being assessed. To be able to assess the latter it is essential that the substance is properly described and any significant impurities are identified.

Interpretation of data

In some cases the dose (concentration) - response (effect) relationship is not known, the duration of a test may be different from that of standard tests or the test parameters may not be comparable to those used in standard tests, for example investigations of photosynthesis, of behaviour, investigations on a cellular or a subcellular level. Expert judgement must therefore be used to determine whether such data can be interpreted for use in the assessment.

Short-term L(E)C50 and long-term NOEC values are used in the effects assessment. Guidance is given in **Table 15** with respect to the derivation of L(E)C50 and NOEC values. However, results from ecotoxicological studies may also be reported using other conventions and expressions of effect. QSARs may be helpful in assessing long-term aquatic toxicity data from very hydrophobic organic chemicals such as PCBs. Long-term tests with such chemicals are difficult to perform because of their low water solubility and the difficulty of maintaining stable test concentrations. Also, it may take a very long time to reach steady state in the test organisms due to their low elimination rate. By comparing the test result with the “minimum toxicity” obtained from a QSAR based on the log Kow of the compound, insight can be gained into the validity of the test result (see Chapter 4 on the “Use of QSARs”).

Further details on the evaluation of the adequacy of data are to be found in Appendix III. Special guidance for metals and metal compounds, petroleum substances and ionisable substances is given in Appendix VIII, IX and XI, respectively.

3.2.2 Quantitative Structure-Activity Relationships

Reliable QSAR estimates for fish, Daphnia and algal toxicity are available for chemicals with a non-specific mode of action. These estimates can be used to assist in data evaluation and/or to contribute to the process of deciding whether further testing is necessary to clarify an endpoint of concern and if so, to optimise the testing strategy, where appropriate. Chapter 4 (Use of QSARs) gives full details on the use of QSAR estimates within the testing strategy for:

- predicting the toxicity of chemicals with a non-specific mode of action; and
- predicting long-term fish toxicity.

Table 15 Overview of toxicity test endpoints

Short-term studies:

- If a test report does not indicate the L(E)C50 values but the raw data are presented, the L(E)C50 should be calculated, for example by Probit analysis. If only one toxicity value lies between the L(E)C0 and the L(E)C100, the L(E)C50 cannot be calculated by Probit analysis. Instead, the L(E)C50 may be estimated by, e.g., linear regression.
- If results are presented as >L(E)C10 and <L(E)C50 , they can be rated as L(E)C50 while results clearly above a L(E)C50 can only be used as an indication of the short-term toxicity of the chemical considered.

Long-term studies:

- The NOEC (no observed effect concentration) is defined as "the highest concentration tested at which the measured parameter shows no significant inhibition" (OECD 201, 1984a) or the test concentration immediately below the LOEC (OECD 210, 1984g). There has to be a concentration-effect relationship. In the past, the NOEC was determined directly from the concentration-effect curve by consideration of the deviation of the control (e.g. 10%) or it was derived on the basis of ANOVA (analysis of variance) and a subordinate test (e.g. Dunett's). The preconditions for the use of ANOVA have to be fulfilled (normal distribution, homogeneous variances). This method to derive the NOEC with the ANOVA is criticised (Pack, 1993, prepared for OECD). The OECD report recommends the calculation of the EC_X point as a preferable alternative (see footnote *). In older investigations, it may be difficult to find out how the NOEC was generated unless test reports or raw data are available.
- A LOEC (lowest observed effect concentration) stands for the lowest concentration where an effect has been observed. It may therefore not be used as a NOEC. In case only a LOEC is given in the report, it can be used to derive a NOEC with the following procedures:
  - LOEC > 10 and < 20% effect: NOEC can be calculated as LOEC/2.
  - LOEC $\geq$ 20% effect and a distinct effect relationship: the EC10 is calculated or extrapolated and regarded as the NOEC.

  If the effect percentage of the LOEC is unknown no NOEC can be derived.
- MATC (maximal acceptable toxicant concentration): In aquatic toxicity the MATC is often calculated. This is the geometric mean of the NOEC and the LOEC. If in the test report only the MATC is presented, the MATC can be divided by $\sqrt{2}$ to derive a NOEC.
- An EC10 for a long-term test which is obtained by extrapolation using appropriate statistics (e.g. Probit analysis) can be considered as a NOEC. This procedure is used if no NOEC is available.
- It should be noted that in the case of algae studies, which are actually multigeneration studies, it is generally accepted that a 72-hour (or longer) EC50 value may be considered as equivalent to a short-term result and that a 72-hour (or longer) NOEC value can be considered as a long-term result.

* "If the reliability in an experiment is relatively high, the corresponding sensitivity of the statistical analysis will be relatively low. Only large differences from the control can then be detected. Consequently, the resulting NOECs can themselves correspond to large and potentially biologically important magnitudes of effect." (Pack, 1993). A concentration where there is a clear effect cannot be regarded as a NOEC. Additionally, the level of the NOEC value depends on the number of test concentrations, range of concentrations and dilution factors. At present, alternatives for the NOEC have been proposed (Pack, 1993; Hoekstra et al., 1993). The advantage of these methods is that information from the whole concentration-effect relationship is taken into account. These methods result in an EC_x, where x is a low effect percentile (e.g. 5-20%). It makes results from different experiments more comparable than NOECs. Currently, the use of the NOEC or the EC_x point estimates are being discussed (Pack, 1993).

3.3 EFFECTS ASSESSMENT FOR THE AQUATIC COMPARTMENT

3.3.1 Calculation of PNEC

For the aquatic environment, a PNEC is derived that, if not exceeded, ensures an overall protection of the environment. Certain assumptions are made concerning the aquatic environment which allow, however uncertain, an extrapolation to be made from single-species short-term toxicity data to ecosystem effects. It is assumed that:

- ecosystem sensitivity depends on the most sensitive species, and;
- protecting ecosystem structure protects community function.

These two assumptions have important consequences. By establishing which species is the most sensitive to the toxic effects of a chemical in the laboratory, extrapolation can subsequently be based on the data from that species. Furthermore, the functioning of any ecosystem in which that species exists is protected provided the structure is not sufficiently distorted as to cause an imbalance. It is generally accepted that protection of the most sensitive species should protect structure, and hence function.

For most substances, the pool of data from which to predict ecosystem effects is very limited as, in general, only short-term toxicity data are available. In these circumstances, it is recognised that, while not having a strong scientific validity, empirically derived assessment factors must be used. Assessment factors have also been proposed by the US EPA and OECD (1992d). In applying such factors, the intention is to predict a concentration below which an unacceptable effect will most likely not occur. It is not intended to be a level below which the chemical is considered to be safe. However, again, it is likely that an unacceptable effect will not occur.

In establishing the size of these assessment factors, a number of uncertainties must be addressed to extrapolate from single-species laboratory data to a multi-species ecosystem. These areas have been adequately discussed in other papers, and may best be summarised under the following headings:

- intra- and inter-laboratory variation of toxicity data;
- intra- and inter-species variations (biological variance);
- short-term to long-term toxicity extrapolation;
- laboratory data to field impact extrapolation (additive, synergistic and antagonistic effects from the presence of other substances may also play a role here).

The size of the assessment factor depends on the confidence with which a PNECwater can be derived from the available data. This confidence increases if data are available on the toxicity to organisms at a number of trophic levels, taxonomic groups and with lifestyles representing various feeding strategies. Thus lower assessment factors can be used with larger and more relevant datasets than the base-set data. Calculation of a PNEC using assessment factors is described in Section 3.3.1.1.

If a large data set from long-term tests for different taxonomic groups is available statistical extrapolation methods may be used to derive a PNEC (Section 3.3.1.2.). In general, it is assumed that sufficient test data for use of statistical extrapolation methods will only be available for relatively few substances and that these data will be primarily fresh water and terrestrial toxicity data. Therefore, the use of statistical extrapolation methods is only described for these two

environments but in case enough data are available, they may be used also for other environments.

3.3.1.1 Calculation of PNEC using assessment factors

The proposed assessment factors are presented in **Table 16.**

When only short-term toxicity data are available, an assessment factor of 1000 will be applied on the lowest L(E)C50 of the relevant available toxicity data, irrespective of whether or not the species tested is a standard test organism (see notes to **Table 16**). A lower assessment factor will be applied on the lowest NOEC derived in long-term tests with a relevant test organism.

For some compounds, a large number of validated short-term L(E)C50 values may be available. Therefore, it is proposed to calculate the geometric mean if more than one L(E)C50 value is available for the same species and end-point. Prior to calculating the geometric mean an analysis of test conditions must be carried out in order to find out why differences in response were present.

The algal growth inhibition test of the base-set is, in principle, a multigeneration test. However, for the purposes of applying the appropriate assessment factors, the EC50 is treated as a short-term toxicity value. The NOEC from this test may be used as an additional NOEC when other long-term data are available. In general, an algal NOEC should not be used unsupported by long-term NOECs of species of other trophic levels. However, if the short-term algal toxicity test is the most sensitive of the short-term tests, the NOEC from this test should be supported by the result of a test on a second species of algae.

Microorganisms representing a further trophic level may only be used if non-adapted pure cultures were tested. The investigations with bacteria (e.g. growth tests) are regarded as short-term tests. Additionally, blue-green algae should be counted among the primary producers due to their autotrophic nutrition.

The assessment factors presented in **Table 16** below should be considered as general factors that under certain circumstances may be changed. In general, justification for changing the assessment factor could include one or more of the following:

- evidence from structurally similar compounds (Evidence from a closely related compound may demonstrate that a higher or lower factor may be appropriate);
- knowledge of the mode of action including endocrine disrupting effects (Some substances, by virtue of their structure, may be known to act in a non-specific manner);
- the availability of test data from a wide selection of species covering additional taxonomic groups other than those represented by the base-set species;
- the availability of test data from a variety of species covering the taxonomic groups of the base-set species across at least three trophic levels. In such a case the assessment factors may only be lowered if these multiple data points are available for the most sensitive taxonomic group.

Specific comments on the use of assessment factors in relation to the available data set are given in the notes below **Table 16**.

Table 16 Assessment factors to derive a $PNEC_{aquatic}$

Available data	Assessment factor
At least one short-term L(E)C50 from each of three trophic levels of the base-set (fish, Daphnia and algae)	1000 a)
One long-term NOEC (either fish or Daphnia)	100 b)
Two long-term NOECs from species representing two trophic levels (fish and/or Daphnia and/or algae)	50 c)
Long-term NOECs from at least three species (normally fish, Daphnia and algae) representing three trophic levels	10 d)
Species sensitivity distribution (SSD) method	5-1 (to be fully justified case by case) e)
Field data or model ecosystems	Reviewed on a case by case basis f)

Notes to Table 16:

a) The use of a factor of 1000 on short-term toxicity data is a conservative and protective factor and is designed to ensure that substances with the potential to cause adverse effects are identified in the effects assessment. It assumes that each of the uncertainties identified above makes a significant contribution to the overall uncertainty. For any given substance there may be evidence that this is not so, or that one particular component of the uncertainty is more important than any other. In these circumstances it may be necessary to vary this factor. This variation may lead to a raised or lowered assessment factor depending on the available evidence. A factor lower than 100 should not be used in deriving a $PNEC_{water}$ from short-term toxicity data except for substances with intermittent release (see Section 3.3.2).
There are cases where the base-set is not complete: e.g. for substances that are produced at <1 t/a (notifications according to Annex VII B of Directive 92/32). At the most the acute toxicity for Daphnia is determined. In these exceptional cases, the PNEC should be calculated with a factor of 1000.
Variation from a factor of 1000 should not be regarded as normal and should be fully supported by accompanying evidence.

b) An assessment factor of 100 applies to a single long-term NOEC (fish or Daphnia) if this NOEC was generated for the trophic level showing the lowest L(E)C50 in the short-term tests.
If the only available long-term NOEC is from a species (standard or non-standard organism) which does not have the lowest L(E)C50 from the short-term tests, it cannot be regarded as protective of other more sensitive species using the assessment factors available. Thus the effects assessment is based on the short-term data with an assessment factor of 1000. However, the resulting PNEC based on short-term data may not be higher than the PNEC based on the long-term NOEC available.
An assessment factor of 100 applies also to the lowest of two long-term NOECs covering two trophic levels when such NOECs have not been generated from that showing the lowest L(E)C50 of the short-term tests. This should, however, not apply in cases where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C50 of the short-term tests.

c) An assessment factor of 50 applies to the lowest of two NOECs covering two trophic levels when such NOECs have been generated covering that level showing the lowest L(E)C50 in the short-term tests. It also applies to the lowest of three NOECs covering three trophic levels when such NOECs have not been generated from that trophic level showing the lowest L(E)C50 in the short-term tests. This should however not apply in cases where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C50 of the short-term tests.

d) An assessment factor of 10 will normally only be applied when long-term toxicity NOECs are available from at least three species across three trophic levels (e.g. fish, Daphnia, and algae or a non-standard organism instead of a standard organism).
When examining the results of long-term toxicity studies, the PNECwater should be calculated from the lowest available NOEC. Extrapolation to the ecosystem effects can be made with much greater confidence, and thus a reduction of the assessment factor to 10 is possible. This is only sufficient, however, if the species tested can be considered to represent one of the more sensitive groups. This would normally only be possible to determine if data were available on at least three species across three trophic levels.
It may sometimes be possible to determine with high probability that the most sensitive species has been examined, i.e. that a further long-term NOEC from a different taxonomic group would not be lower than the data already available. In those circumstances, a factor of 10 applied to the lowest NOEC from only two species would also be appropriate. This is particularly important if the substance does not have a potential to bioaccumulate. If it is not possible to make this judgement, then an assessment factor of 50 should be applied to take into account any interspecies variation in sensitivity. A factor of 10 cannot be decreased on the basis of laboratory studies.

e) Basic considerations and minimum requirements as outlined in Section 3.3.1.2.

f) The assessment factor to be used on mesocosm studies or (semi-) field data will need to be reviewed on a case-by-case basis.

For compounds with a high log Kow no short-term toxicity may be found. Also, even in long-term tests this may be the case or steady state may still not have been reached. In fish tests for non-polar narcotics, the latter can be substantiated by the use of long-term QSARs (see Section 3.2.1.2 and Chapter 4 on the Use of QSARs). Use of a higher assessment factor can be considered in such cases where steady state does not seem to have been reached.

A long-term test has to be carried out for substances showing no toxicity in short-term tests if the log Kow > 3 (or BCF > 100) and if the PEClocal/regional is > 1/100th of the water solubility (see Section 4.6). The long-term toxicity test should normally be a Daphnia test to avoid unnecessary vertebrate testing. The NOEC from this test can then be used with an assessment factor of 100. If in addition to the required long-term test a NOEC is determined from an algal test of the base-set, an assessment factor of 50 is applied.

3.3.1.2 Calculation of PNEC using statistical extrapolation techniques

The effect assessment performed with assessment factors can be supported by a statistical extrapolation method if the database on Species Sensitivity Distributions (SSDs) is sufficient for its application. If a large data set from long-term tests for different taxonomic groups is available (OECD, 1992d), statistical extrapolation methods may be used to derive a PNEC. The main underlying assumptions of the statistical extrapolation methods are as follows (OECD, 1992d):

- the distribution of species sensitivities follows a theoretical distribution function;
- the group of species tested in the laboratory is a random sample of this distribution.

In general, the methods work as follows: long-term toxicity data are log transformed and fitted according to the distribution function and a prescribed percentile of that distribution is used as criterion. Several distribution functions have been proposed. The US EPA (1985) assumes a log-triangular function, Kooijman (1987) and Van Straalen and Denneman (1989) a log-logistic function, and Wagner and Løkke (1991) a log-normal function. Aldenberg and Slob (1993) refined the way to estimate the uncertainty of the 95th percentile by introducing confidence levels.

The approach of statistical extrapolation is still under debate and needs further validation. An advantage of these methods is that they use the whole sensitivity distribution of species in an ecosystem to derive a PNEC instead of taking always the lowest long-term NOEC. However, such methods could also be criticised. Among the most common drawbacks, the reasons put forward are: the lack of transparency by using this method compared to the standard approach, the question of representativity of the selected test species, the comparability of different endpoints, the arbitrary choice of a specific percentile and a statistical confidence level etc.

In response to these concerns it has been seen as necessary to provide some guidance on when and how to use such methods. What is proposed below has been discussed during an Expert Consultation Workshop on Statistical Extrapolation Techniques for Environmental Effects Assessments, in London on 17-18th January 2001 (EC, 2001). Although the primary objective of this workshop was focused on how statistical extrapolation techniques might be used to derive PNECs in the assessments of metals and their compounds, the general principles outlined here should be also applicable for other substances.

Input data

The methods should be applied on all reliable available NOECs from chronic/long-term studies, preferably on full life-cycle or multi-generation studies. NOECs are derived according to previous considerations (**Table 15**).

Which taxonomic groups

It is important to include all available information on the mode of action of the chemical, in order to evaluate the need to include possible other (sensitive) taxonomic groups or exclude possible over-representation of certain taxonomic groups, realising that the mode of action may differ between short-term effects and long-term effects and between taxonomic groups. The minimum species requirements when using the Species Sensitivity Distribution method are:

- fish (species frequently tested include salmonids, minnows, bluegill sunfish, channel catfish, etc.);
- a second family in the phylum Chordata (fish, amphibian, etc.);
- a crustacean (e.g. cladoceran, copepod, ostracod, isopod, amphipod, crayfish etc.);
- an insect (e.g. mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge, etc.);
- a family in a phylum other than Arthropoda or Chordata (e.g. Rotifera, Annelida, Mollusca, etc.);
- a family in any order of insect or any phylum not already represented;
- algae;
- higher plants.

It is recognised that for some of the taxa mentioned above, no internationally standardised test guidelines for long-term tests are currently available. The applicability of existing test data and the fulfilment of the above requirements thus need to be assessed on a case-by-case basis. There is a need to evaluate additional information in order to assess how relevant and representative the list of taxonomic groups is to the risk assessment scenario being investigated.

Minimal sample size (number of data)

Confidence can be associated with a PNEC derived by statistical extrapolation if the database contains at least 10 NOECs (preferably more than 15) for different species covering at least 8 taxonomic groups.

Deviations from these recommendations can be made, on a case-by-case basis, through consideration of sensitive endpoints, sensitive species, mode of toxic action and/or knowledge from structure-activity considerations.

How to deal with multiple data for one species?

Where appropriate and possible, a pre-selection of the data should be performed in relation to realistic environmental parameters for Europe (e.g. hardness of water, pH, organic matter and/or temperature). The full database should be carefully evaluated to extract information (e.g., on sensitive endpoints), which may be lost when "averaging" the data to a single value.

The test data applicable to the most sensitive endpoint should be taken as representative for the species. In this context, demographic parameters can be used as endpoints, as can bio-markers if they are toxicologically relevant in terms of population dynamics.

Multiple values for the same endpoint with the same species should be investigated on a case-by-case basis, looking for reasons for differences between the results. For equivalent data on the same end-point and species, the geometric mean should be used as the input value for the calculation. If this is not possible, perhaps because valid results are considered to be too variable, then grouping and combining the values, e.g. by pH ranges, and using reduced numbers of values should be considered. The effects that these different treatments have on the derived value (and on the resulting risk characterisation) should be investigated and discussed.

Where it is considered that the results are limited to certain conditions (e.g. not appropriate for low pH conditions) then these limitations should be explained. The values derived from different treatments of the data may be useful to indicate sensitive regions.

Fit to a distribution

Different distributions like e.g. log-logistic, log-normal or others may be used (Aldenberg and Jaworska, 2000, Aldenberg and Slob, 1993). The log-normal distribution is a pragmatic choice from the possible families of distributions because of the available description of its mathematical properties (methods exist that allow for most in depth analyses of various uncertainties).

The Anderson–Darling goodness of fit test can be used in addition to the Kolmogorov-Smirnov-test, as a criterion for the choice of a parametric distribution for comprehensive data sets, because it gives more weight to the tails of the distribution. A lack of fit may be caused by very different factors. One common factor seems to be the inclusion of several NOECs for species tested in a single laboratory, where the same test concentrations were used for all species. The statistical determination of the NOEC can lead to the same value being obtained for several species, showing up as a vertical row of NOECs in the cumulative distribution plots. Another reason for lack of fit is a possible bimodality of the SSD, due to a specific mode of action of the tested substance towards only some taxonomic groups of species.

Whatever the fit to a distribution, results should be discussed in regards to the graphical representation of the species distribution and the different p values that were obtained with each test. Finally, any choice of a specific distribution function should be clearly explained.

If the data do not fit any distribution, the left tail of the distribution (the lowest effect concentrations) should be analysed more carefully. If a subgroup of species can be identified as particularly sensitive and if the number of data on this subgroup is sufficient, the distribution can be fit to this subgroup. In case of lack of fit, the SSD method should not be used.

Estimated parameter

For pragmatic reasons it has been decided that the concentration corresponding with the point in the SSD profile below which 5% of the species occur should be derived as an intermediate value in the determination of a PNEC. A 50% confidence interval (c.i.) associated with this concentration should also be derived.

Estimation of the PNEC

The PNEC is calculated as:

$$PNEC = \frac{5\%SSD(50\%c.i.)}{AF} \tag{69}$$

AF is an appropriate assessment factor between 5 and 1, reflecting the further uncertainties identified. Lowering the AF below 5 on the basis of increased confidence needs to be fully justified. The exact value of the AF must depend on an evaluation of the uncertainties around the derivation of the 5th percentile. As a minimum, the following points have to be considered when determining the size of the assessment factor:

- the overall quality of the database and the endpoints covered, e.g., if all the data are generated from "true" chronic studies (e.g., covering all sensitive life stages);
- the diversity and representativity of the taxonomic groups covered by the database, and the extent to which differences in the life forms, feeding strategies and trophic levels of the organisms are represented;
- knowledge on presumed mode of action of the chemical (covering also long-term exposure);
- statistical uncertainties around the 5th percentile estimate, e.g., reflected in the goodness of fit or the size of confidence interval around the 5th percentile, and consideration of different levels of confidence (e.g. by a comparison between the 5% of the SSD (50%) with the 5% of the SSD (95%));
- comparisons between field and mesocosm studies, where available, and the 5th percentile and mesocosm/field studies to evaluate the laboratory to field extrapolation.

A full justification should be given for the method used to determine the PNEC.

Further recommendations

NOEC values below the 5% of the SSD need to be discussed in the risk assessment report. For example if all such NOECs are from one trophic level, then this could be an indication that a particular sensitive group exists, implying that some of the underlying assumptions for applying the statistical extrapolation method may not be met;

The deterministic PNEC should be derived by applying the "standard" Assessment Factor Approach on the same database;

If mesocosm studies are available, they should also be evaluated and a PNEC derived following the TGD according to the standard method (deterministic approach).

The various estimates of PNEC should be compared and discussed and the final choice of a PNEC be based on this comparison.

3.3.2 Effects assessment for substances with intermittent release

For substances subject to intermittent release (see Section 2.3.3.4 for the definition of intermittent release), a single exposure event may be of only short duration. At least for dynamic systems such as rivers, the likelihood of long-term effects arising from such exposure is low, the principal risk being that of short-term toxic effects. Thus, the risk assessment should be based on a no-effect-concentration for intermittent release. In extrapolating to such a PNECwater, intermittent, therefore, generally only short-term effects need to be considered. It is therefore proposed that, to derive a PNECwater, intermittent for such situations, an assessment factor of 100 be normally applied to the lowest L(E)C50 of at least three short-term tests from three trophic levels. The assessment factor is designed to take account of the uncertainty that exists in extrapolating from the results of short-term laboratory toxicity tests to short-term effects that can be anticipated in the ecosystems.

In undertaking such an extrapolation, due account is taken of the biological variables of intra- and inter-species toxicity, as well as the general uncertainties in predicting ecosystem effects from laboratory data. This extrapolation should be carried out with care. Some substances may be taken up rapidly by aquatic organisms and this can lead to delayed effects even after exposure has ceased. This will generally be taken into account by the assessment factor of 100 but there may be occasions when a higher or lower factor would be appropriate. For substances with a potential to bioaccumulate the lowered assessment factor of 100 may not always be sufficient to provide adequate protection. For substances with a known non-specific mode of action, inter-species variations may be low. In such cases, a lower factor may be appropriate. In no case should a factor lower than 10 be applied to a short-term L(E)C50 value.

3.4 EFFECTS ASSESSMENT FOR MICROORGANISMS IN SEWAGE TREATMENT PLANTS (STP)

Since chemicals may cause adverse effects on microbial activity in STPs it is necessary to derive a $PNEC_{microorganisms}$ (see Section 2.3.7). The $PNEC_{microorganisms}$ will be used for the calculation of the PEC/PNEC ratio concerning microbial activity in STPs. Current test systems for measuring the effect of chemicals on microbial activity have different endpoints and different levels of sensitivity. A number of internationally accepted test systems exist (cf. table below). Available data (e.g. UBA, 1993; Reynolds et al., 1987) suggest the following order of increasing sensitivities among particular test systems: respiration inhibition test (EU Annex V C.11; OECD 209, 1984f) < inhibition control in base-set tests < growth inhibition test with P. putida < inhibition of nitrification.

In general, short-term measurements in the order of hours (e.g. 10 h) are preferred, in accordance with the retention time in a STP. Information available on the toxicity for microorganisms has also to be relevant for the endpoint considered, i.e. microbial degradation activity in a STP. Test systems such as the respiration inhibition test and the nitrification inhibition test can be used. Respiration tests using a mixed inoculum are considered more relevant than respiration inhibition tests using a single-species inoculum.

The assumption that the substance under investigation is not inhibitory to the microorganisms when dosed in the test system is implicit in ready biodegradability testing (i.e., EU Annex V C.4A-F, OECD 301A-F, 1992f). Reynolds et al. (1987) report that microbial EC50 values determined for test substances using a variety of tests (Annex V C.11, OECD 209, 1984f, Annex V C.4F, Closed Bottle Test, Growth Inhibition) were found to be inhibitory in ready

biodegradability tests (Annex V C.4C,F,E,B; OECD 301B,C,D,E, 1992f). No-effect or EC0 values were 1.5 to 10 times lower than the corresponding EC50 values. The authors recommend as a provisional rule that biodegradation testing should therefore be conducted at one-tenth of the EC50 concentration to ensure that a "probable non-inhibitory level" is employed in biodegradation testing. It would, therefore, seem appropriate to consider the test concentration from a positive ready biodegradability test to be an acceptable alternative to a NOEC obtained from a microbial toxicity test for the purposes of determining a $PNEC_{microorganisms}$. This is particularly the case if domestic sludge is used as the source of microorganisms and if there is no indication of toxicity for the test concentration, e.g. due to other available test results. Similarly, data from inherent biodegradability testing may also prove useful. However, some additional issues have to be considered:

Only Ready Biodegradability Tests (RBT) relying on continuous monitoring, i.e. the MITI I test (EU Annex V C.4F; OECD 301C, 1992f) and the Manometric Respirometry test (EU Annex V C.4D; OECD 301F, 1992f), are considered reliable for observing the effects of a chemical on the inoculum, i.e. activated sludge diluted by factors ranging from ca. 100 to 1000. In parallel to the test itself, a toxicity control is run in extra bottles containing both the test chemical and a reference chemical that is easily degraded in the system. If for that purpose sodium acetate is used, the toxic effect is most often manifest as a delayed mineralisation of the substance. However, even if the vast majority of microorganisms are initially killed in the test system, such a delay may only be in the order of a few hours or days before rapid mineralisation of sodium acetate takes place. If measurements are carried out only weekly, which is the case in most RBT's, a delay in mineralisation of sodium acetate of only a few days may not be detected, leading erroneously to the conclusion that the test chemical is not inhibitory. Sodium benzoate may provide an acceptable alternative to sodium acetate when an inhibitory control test (i.e. the official term, not 'toxicity test') is performed with an RBT method that is not based on continuous monitoring, because mineralisation of benzoate occurs at a much slower rate.

Subject to expert judgement, consideration of data from biodegradation/removal studies using the laboratory/pilot scale Activated Sludge Simulation, Continuous Activated Sludge or Aerobic Sewage Treatment Coupled-Units tests (OECD 303A, 2001b; ISO-11733) may also prove useful in any consideration of $PNEC_{microorganisms}$. These tests are laboratory scale models for simulation of activated sludge, representing realistic approximation to actual conditions within full scale STPs. A NOEC from well-conducted simulation studies using domestic activated sludge would correspond to the concentration of the chemical substance that does not perturb the proper functioning of the Continuous Activated Sludge unit with regard to performance parameters such as:

- test substance elimination;
- COD removal;
- nitrification;
- denitrification;
- phosphorus removal;
- effluent quality etc.

when compared to a parallel non-dosed control.

Additionally, the results from tests with ciliated protozoa can be used for deriving a $PNEC_{microorganisms}$. In this case protozoa have to be regarded as additional species, not as an additional trophic layer. Ciliated protozoa, constituting the most important class of protozoa in STPs, are, except for certain industrial plants, important for their functioning. The toxicity data

for ciliates are considered to be supplementary to the data for activated sludge or specific bacteria, i.e. no correlation exists between activated sludge and ciliate test results, neither are ciliates consistently more sensitive. The data from one ciliate species are representative for other ciliates, i.e. test data from species not dominant or not present in STPs can serve as basis for the PNEC-derivation. The function of the protozoa in STP is correlated to their growth. Therefore, values from ciliate growth inhibition tests, preferably with *Tetrahymena* (cf. OECD, 1998a), are relevant for the risk assessment for STPs. Tests using other characteristics (e.g. ciliary motion, cell movement, etc.) should not serve as a basis for the PNEC-derivation.

Often information may also be present on individual bacterial species such as from tests with *Vibrio fischeri* (used in the MICROTOX test), *Pseudomonas putida*, *Pseudomonas fluorescens* and even *Escherichia coli*. These tests must be considered as less relevant. The tests with *P. fluorescence* and *E. coli* (Bringmann and Kühn, 1960) cannot be used for determination of the $PNEC_{microorganisms}$ as they use glucose as a substrate. Likewise, the MICROTOX test cannot be used as it uses a saltwater species. Results of the cell multiplication inhibition test with *P. putida* (Bringmann and Kühn, 1980) should only be used for calculation of the $PNEC_{microorganisms}$ in cases where no other test results employing mixed inocula are available.

In general, the aim of the assessment is the protection of the degradation and nitrification functions and process performance and efficiency of domestic and industrial STPs – as also influenced by protozoan populations. The toxicity of a substance to microorganisms in a STP is assessed by comparing the concentration of a substance in STP aeration tank with the microbial effect concentration data for that substance (see also Section 2.3.7.1). If the substance under consideration is relevant for industrial and municipal STPs the toxicity assessment should be conducted for both kinds of STPs separately. A $PNEC_{microorganisms}$ should be obtained as a first step in the effects assessment for microorganisms in both domestic and industrial sewage treatment plants. The $PNEC_{microorganisms}$ is usually derived from results obtained in the most sensitive test system available, regardless of whether this is a test with activated sludge, relevant bacteria or ciliated protozoa:

- the $PNEC_{microorganisms}$ is set equal to a NOEC from a test performed with 'specific bacterial populations' like nitrifying bacteria or *P. putida* or from a growth inhibition test performed with ciliated protozoa. An EC50 from this test is divided by an assessment factor of 10;
- a NOEC or EC10 from other test systems like the respiration inhibition test (EU Annex V C.11; OECD 209, 1984f) is divided by an assessment factor of 10. An EC50 from this test is divided by an assessment factor of 100;
- the lowest value is selected as the $PNEC_{microorganisms}$.

There may be cases in which the lowest $PNEC_{microorganisms}$ does not correspond to the effect value of the most sensitive test system because different AF (100 or 10) are applied to the different test systems. In these cases expert judgement should be used to decide which effect value is appropriate for the calculation of the $PNEC_{microorganisms}$. Usually the effect value of the most sensitive test system should be used as a basis for the calculation of $PNEC_{microorganisms}$ employing the appropriate AF.

Table 17 provides a complete listing of the test systems mentioned above, effect concentrations that are determined using them and the corresponding assessment factors.

Table 17 Test systems for derivation of $PNEC_{microorganisms}$

Test	Available value	Assessment factor
Respiration inhibition tests EU Annex V C.11; OECD 209 (1984f) ISO 8192 (1986)	NOEC or EC10	10
	EC50	100
Inhibition control in standardised biodegradation tests - Ready biodegradability tests EU Annex V C.4 A-F; OECD 301A-F (1992f) 92/69/EEC C4 (1992) ISO-7827 (1994), -9439 (1999), -10707 (1994), -9408 (1999) - Inherent biodegradability tests EU Annex V C.9; OECD 302 B-C (1981d-1992g) 88/302/EEC (1988) ISO-9888 (1999)	The tested concentration at which toxicity to the inoculum can be ruled out with sufficient reliability (cf. corresponding text section above) could be considered as a NOEC for the toxicity to microorganisms of a STP	10
Inhibition of nitrification ISO-9509 (1989)	NOEC or EC10	1
	EC50	10
Ciliate growth inhibition tests (preferably with *Tetrahymena*, cf. OECD, 1998a) [1)]	NOEC or EC10	1
	EC50	10
Activated sludge growth inhibition tests ISO-15522	NOEC or EC10	10
	EC50	100
Pilot scale activated sludge simulation tests OECD 303A (2001b) ISO-11733	Based on case-by-case expert judgement, the tested concentration not impairing proper functioning of the CAS [2)] unit could be considered as NOEC for microorganisms in STPs	Case-by-case down to 1
Growth inhibition test with *Pseudomonas putida* NF EN ISO 10712 (1995)	NOEC or EC10	1
	EC50	10
(Bringmann and Kühn, 1980)	to be used if no other tests are available	
Pseudomonas fluorescens (Bringmann and Kühn, 1960)	Not usable as it uses glucose as substrate	
Escherichia coli (Bringmann and Kühn, 1960)	Not usable as it uses glucose as substrate	
Vibrio fischeri (MICROTOX) NF EN ISO 11348-1, -2, -3 (1999)	Not relevant for STP as the bacterium is a saltwater species	

Notes to Table 17:

1) Ciliate testing would be required as the guideline becomes available
2) CAS: Continuous Activated Sludge

If on the basis of the $PNEC_{microorganisms}$ derived using the procedures described above the PEC/PNEC ratio for industrial / domestic sewage treatment plants is above 1, the following procedure is proposed for refining the $PNEC_{microorganisms}$:

- If on the basis of a test with nitrifying bacteria, a PEC/PNEC ratio above 1 is derived for a specific industrial STP, a revised $PNEC_{microorganisms}$ for this specific site can be derived from a nitrification inhibition test using sludge from this site's STP. The revised $PNEC_{microorganisms}$ for a specific industrial STP is derived from this test using the assessment factors described for nitrifying bacteria. For domestic STPs a revision of the PNEC is not possible in this way - sludge from one STP can not be regarded as being representative (in comparison with the single species test) of all domestic STPs with respect to the nitrifying activity;
- If on the basis of a respiration inhibition test, a PEC/PNEC ratio above 1 is derived for a specific industrial STP, a revised $PNEC_{microorganisms}$ for this specific STP can be derived from a respiration inhibition test using sludge from this site's STP (the result from such a test is sometimes already available). A revised $PNEC_{microorganisms}$ for a specific industrial STP is derived from these tests using the assessment factors described above for respiration inhibition tests. A $PNEC_{microorganisms}$ for domestic STPs can not be derived on the basis of results from respiration tests that use industrial sludge as the source of inoculum;
- If on the basis of a respiration inhibition test, a standardised biodegradation test or an activated sludge growth inhibition or simulation test, a PEC/PNEC ratio above 1 is derived for a specific industrial sewage treatment plant, a revised $PNEC_{microorganisms}$ for this site can be derived from an appropriate pilot scale simulation test using activated sludge from the site's STP as a source of inoculum;
- If on the basis of a single species test with ciliated protozoa a PEC/PNEC ratio above 1 is derived for municipal or industrial sewage treatment plants, a test reflecting the integrity of the native ciliate population in (industrial or domestic) sewage sludge is necessary. The exception to this is where it can be shown that for the industrial STP under consideration protozoa are not relevant. The ability of the protozoan community to eliminate external bacterial food supply should be considered as a possible endpoint in this test. At present a standard protocol for a test based on ciliated protozoa which can be used to provide data for revising a $PNEC_{microorganisms}$ is not available.

3.5 EFFECTS ASSESSMENT FOR THE SEDIMENT

3.5.1 Introduction

Sediments may act as both a sink for chemicals through sorption of contaminants to particulate matter, and a source of chemicals through resuspension. Sediments integrate the effects of surface water contamination over time and space, and may thus present a hazard to aquatic communities (both pelagic and benthic) which is not directly predictable from concentrations in the water column. Effects on benthic organisms are of concern because they constitute an important link in aquatic food chain and play an important role in the recycling of detritus material. Due to the lack of standardised test methods on, e.g., the role of microorganisms in recycling of detritus material and nutrients, further tests needs to be developed and to be added for guidance in future.

It is unlikely that data for sediment dwelling organisms will be available for new substances. To date, only a few tests with sediment organisms have been conducted in Europe with existing substances. However, research is in progress in this field in various countries. The selection of

representative organisms and the selection of standardised sediments are still being discussed. Various approaches (e.g. equilibrium partitioning, interstitial water quality, spiked sediment toxicity, tissue residue, derived sediment quality criteria and standards) are being developed to investigate the effects that chemicals have on sediment and sediment organisms (OECD, 1992b). Only whole-sediment tests using benthic organisms are suitable for a realistic risk assessment of the sediment compartment. It is only by using such tests that it is possible to adequately address all routes of exposure. A $PNEC_{sed}$ can be derived from these tests that can be compared with the predicted concentration in the sediment (PEC_{sed}) (based on measured or estimated values). Test procedures are described in ASTM (1990 a–e), ASTM (1991, 1993 & 1994) and Burton (1991 & 1992). No finalised international guidelines for whole-sediment tests are available. However, a draft OECD guideline for a chironomid toxicity test using spiked sediment exists (OECD, 2001e). In addition OECD has prepared a detailed review paper on aquatic ecotoxicity tests including sediment test methods (OECD, 1998a). Examples of sediment toxicity tests for which protocols are available are listed in Appendix VI.

Statistical extrapolation methods for calculation of PNEC for sediment organisms could be used when sufficient data are available (cf. Section 3.3.1.2.). Further guidance needs to be developed in future.

3.5.2 Strategy for effects assessment for sediment organisms

Substances that are potentially capable of depositing on or sorbing to sediments to a significant extent have to be assessed for toxicity to sediment-dwelling organisms. In addition, marine sediment effects assessment is necessary for substances that are known to be persistent in marine waters, and may accumulate in sediments over time. In general, substances with a $K_{oc} < 500 – 1000$ L/kg are not likely sorbed to sediment (SETAC, 1993). To avoid extensive testing of chemicals a log K_{oc} or log K_{ow} of ≥ 3 can be used as a trigger value for sediment effects assessment.

For most chemicals the number of toxicity data on sediment organisms will be limited. For the initial risk assessment, normally no effect data from tests with sediment organisms will be available. Therefore, the equilibrium partitioning method is proposed as a screening approach to compensate for this lack of toxicity data. Results from this screening can be used as a trigger for determining whether whole-sediment tests with benthic organisms should be conducted. Tests with benthic organisms using spiked sediment are likely to be necessary if, using the equilibrium partitioning method, a PEC/PNEC ratio > 1 is derived. The test results will enable a more realistic risk assessment of the sediment compartment to be carried out.

Three situations can be distinguished for deriving a $PNEC_{sed}$:

- when no toxicity test results are available for sediment organisms, the equilibrium partitioning method is applied to identify a potential risk to sediment organisms. This method is regarded as “screening approach” and is explained in Section 3.5.3;
- when only acute toxicity test results for benthic organisms are available (at least one) the risk assessment is performed both on the basis of the test result of the most sensitive species using an assessment factor of 1000 and on the basis of the equilibrium partitioning method. The lowest $PNEC_{sed}$ is then used for the risk characterisation;
- when long-term toxicity test data are available for benthic organisms the $PNEC_{sed}$ is calculated using assessment factors for long-term tests and this result should prevail in the risk assessment. This approach is explained in Section 3.5.4.

If no measured data are available, either for the determination of a PEC_{sed} or for the calculation of a $PNEC_{sed}$, no quantitative risk characterisation for sediment can be performed. In this case the assessment conducted for the aquatic compartment will also cover the sediment compartment for chemicals with a log K_{ow} up to 5. For substances with a log K_{ow} > 5, or with a corresponding adsorption or binding behaviour, the PEC/PNEC ratio for the aquatic compartment is increased by a factor of 10. This factor is justified by the fact that the equilibrium partitioning method considers only the exposure via the water phase. The additional factor of 10 on the PEC/PNEC ratio takes into account the possible additional uptake via sediment ingestion (see Section 3.5.3). It has to be borne in mind that even this factor may be insufficient to achieve an appropriate level of protection in case of, for example, ionisable substances.

Table 18 presents an overview of different data configurations and explains how to use them for the risk characterisation for sediment.

Table 18 Requirements for performing a risk characterisation for sediment

Available measured data: PEC_{sed}	Available measured data: $PNEC_{sed}$	Risk characterisation
$C_{pore\ water}$ / —	none	$\frac{C_{pore\ water}}{PNEC_{water}}$
C_{bulk}	none	$\frac{C_{bulk}\ RHO_{susp}}{K_{susp\text{-}water}\ PNEC_{water} \cdot 1000}$
none	$PNEC_{sed}$	$\frac{K_{susp\text{-}water}\ PEC_{water} \cdot 1000}{PNEC_{sed}\ RHO_{susp}}$
$C_{pore\ water}$ / —	$PNEC_{sed}$	$\frac{K_{susp\text{-}water}\ C_{pore\ water} \cdot 1000}{PNEC_{sed}\ RHO_{susp}}$
C_{bulk}	$PNEC_{sed}$	$\frac{C_{bulk}}{PNEC_{sed}}$

where:

$C_{pore\ water}$	concentration in sediment pore water	$[mg \cdot l^{-1}]$	
C_{bulk}	concentration in whole sediment	$[mg \cdot kg_{sed}^{-1}]$	
$K_{susp\ water}$	suspended matter-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	eq. (10)
RHO_{susp}	bulk density of suspended matter	$[kg \cdot m^{-3}]$	eq. (4)

3.5.3 Calculation of PNEC using the equilibrium method

In the absence of any ecotoxicological data for sediment-dwelling organisms, the $PNEC_{sed}$ may be provisionally calculated using the equilibrium partitioning method. This method uses the $PNEC_{water}$ for aquatic organisms and the sediment/water partitioning coefficient as inputs (OECD, 1992b; Di Toro et al., 1991).

In the partitioning method, it is assumed that the:

- sediment-dwelling organisms and water column organisms are equally sensitive to the chemical;
- concentration of the substance in sediment, interstitial water and benthic organisms are at thermodynamic equilibrium: the concentration in any of these phases can be predicted using the appropriate partition coefficients;
- sediment/water partition coefficients can either be measured or derived on the basis of a generic partition method from separately measurable characteristics of the sediment and the properties of the chemical. (For the derivation of the sediment-water partition coefficient and the limits of the calculation methods see Section 2.3.5).

The following formula, which is based on equilibrium partitioning theory, is applied:

$$PNEC_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PNEC_{water} \cdot 1000 \qquad (70)$$

Explanation of symbols

$PNEC_{water}$	Predicted No Effect Concentration in water	$[mg \cdot l^{-1}]$	
RHO_{susp}	bulk density of wet suspended matter	$[kg \cdot m^{-3}]$	eq. (18)
$K_{susp\ water}$	partition coefficient suspended matter water	$[m^3 \cdot m^{-3}]$	eq. (24)
$PNEC_{sed}$	Predicted No Effect Concentration in sediment	$[mg \cdot kg^{-1}]$	

The following qualifying comments apply regardless of whether the $K_{susp\ water}$ is measured or estimated:

- the formula only considers uptake via the water phase. However, uptake may also occur via other exposure pathways like ingestion of sediment and direct contact with sediment. This may become important, especially for adsorbing chemicals, for example those with a log Kow greater than 3. For these compounds the total uptake may be underestimated;
- there is evidence from studies in soil (Belfroid et al., 1995) that the proportion of the total dose remains low for chemicals with a log Kow up to 5. Although it is recognised that in principle results for the soil compartment may not be extrapolated to the sediment compartment, it is considered that the possible underestimation of exposure is acceptable when using the equilibrium partitioning method for chemicals with a log Kow between 3 and 5;
- for compounds with a log Kow greater than 5 (or with a corresponding adsorption or binding behaviour, e.g. ionisable substances) the equilibrium method is used in a modified way.

In order to take uptake via ingestion of sediment into account, the $PEC_{sed}/PNEC_{sed}$ ratio is increased by a factor of 10. It should be borne in mind that this approach is considered only as a screen for assessing the level of risk to sediment dwelling organisms. If with this method a PEC/PNEC ratio > 1 is derived, then tests with benthic organisms using spiked sediment have to be conducted to support a refined risk assessment for the sediment compartment.

3.5.4 Calculation of PNEC using assessment factors

If results from whole-sediment tests with benthic organisms are available the $PNEC_{sed}$ has to be derived from these tests using assessment factors. However, the available sediment tests should be carefully evaluated. Special attention should be given to the pathways through which the test organisms are exposed to the chemical and the test protocol should carefully be checked, whether feeding with unspiked food has possibly reduced exposure via sediment ingestion. For assessing the toxicity of spiked sediment it is necessary to address adequately all possible routes of exposure. Sediment organisms can be exposed via their body surfaces to substances in solution in the overlying water and in the pore water and to bound substances by direct contact or via ingestion of contaminated sediment particles. The route that is most important is strongly influenced by species-specific feeding mechanisms and the behaviour of the organism in, or on, the sediment. Test design parameters can have a bearing on the route of uptake of a substance.

A number of uncertainties have to be addressed (cf. Chapter 3.3.1) in establishing the size of the assessment factors. In contrast to the principle adopted for the aquatic compartment, it is not necessary to have 3 acute sediment tests for the assessment factor of 1000 to be applicable. Results from long-term tests with sub-lethal endpoints such as reproduction, growth, emergence, sediment avoidance and burrowing activity are regarded as most relevant due to the generally long-term exposure of benthic organisms to sediment-bound substances. Consequently, if results from short-term tests with sediment-dwelling organisms are only available (at least one) an assessment factor of 1000 is applied to the lowest value. In addition, the $PNEC_{sed}$ should also be calculated from the $PNEC_{water}$ using the equilibrium-partitioning method. A reduction in the size of the assessment factor should only be accepted if results form long-term tests with sediment-dwelling organisms are available.

The $PNEC_{sediment}$ is derived from the lowest available NOEC/EC10 obtained in long-term tests by application of the following assessment factors (**Table 19**):

Table 19 Assessment factors for derivation of $PNEC_{sed}$

Available test result	Assessment factor
One long-term test (NOEC or EC10)	100
Two long-term tests (NOEC or EC10) with species representing different living and feeding conditions	50
Three long-term tests (NOEC or EC10) with species representing different living and feeding conditions	10

3.6 EFFECTS ASSESSMENT FOR THE TERRESTRIAL COMPARTMENT

3.6.1 Introduction

Chemicals can reach the soil via several routes: application of sewage sludge in agriculture, direct application of chemicals and deposition from the atmosphere. Consequently the possibility of adverse effects has to be assessed. The proposed strategy in this section is based on assessing the effects of chemicals on soil organisms. At the moment no strategy is available to assess possible effects on soil functions such as filtration, buffering capacity and metabolic capacity.

As mentioned in the introduction, the substances discharged into the soil can not only affect the soil organisms but also can influence soil functions. Substances that are hydrophilic and that are readily eluted with the rainwater into the ground water as well as those that geo-accumulate and those that are poorly degradable in soil should be considered with special care. If the substance is a biocide directly applied/emitted to soil, then the methodology referred in the Technical Notes for Guidance in support of Directive 98/8 concerning the placing of biocidal products on the market is recommended (http://ecb.jrc.it/biocides/).

The terrestrial ecosystem comprises of an above-ground community, a soil community and a groundwater community. In this section only effects on soil organisms exposed directly via pore water and/or soil are addressed. It is recognised that the strategy described here must therefore be regarded as provisional. However, reference is made to the strategy for the air compartment (Section 3.7) and for bioaccumulation and secondary poisoning of birds and mammals (Section 3.8). It is currently not possible to carry out effect assessment for the groundwater community because no toxicity data are available. However, ecotoxicity tests with groundwater fauna and microflora have been proposed by Notenboom and Boessenkool (1992) and Van Beelen et al. (1990).

The strategy described below is based on several documents relating to terrestrial effects assessment: OECD (1989), Stavola (1990), Samsøe-Petersen and Pedersen (1994), UBA (1993) and Römbke et al. (1993).

3.6.2 Strategy for effects assessment for soil organisms

Standardised methods exist for the soil compartment but toxicity tests with terrestrial organisms are not yet included in a base set. For new substances toxicity tests with plants and earthworms can be requested at level 1. At level 2 there are, as yet, no specific additional requirements to examine effects on soil organisms. For existing substances data will probably be scarce: for most chemicals the data set will consist of results from short-term tests with for example earthworms and plants. Long-term tests methods are available (e.g. springtails and earthworms) but results from these tests are seldom available for existing substances. For biocides, toxicity tests with terrestrial organisms may be required depending on product type and expected use.

The equilibrium partitioning method can be applied to aquatic data to identify a PNEC for soil organisms. However, this method cannot replace toxicity data for soil organisms and should only be considered as a screen for identifying substances requiring further testing.

In common with the aquatic compartment, the objective of the assessment is to identify substances that present an immediate or delayed danger to the soil communities.

Soil is a complex and heterogeneous medium in which biological processes are occurring. Microorganisms play an important role in degradation processes and the mineralisation of organic matter, allowing nutrients to be re-cycled in the ecosystem. Soil invertebrates are contributing to the recycling of elements and play a significant part in creating and maintaining a good soil structure. Finally, plants are primary producers and provide food for all other heterotrophic organisms. Consequently, the protection of the soil community requires protection of all organisms playing a leading role in establishing and maintaining the structure and the functioning of the ecosystem. The use of results from tests that represent different and significant ecological functions in the soil ecosystem is therefore suggested.

A suite of soil tests should therefore ideally be designed to obtain data relevant to:

- primary producers (plants);
- consumers (for example invertebrates that represent an important group in the soil compartment);
- decomposers (comprising microorganisms that play an important role in foodwebs and nutrients cycling).

Natural soils used in ecotoxicological tests differ in characteristics such as organic matter and clay content, soil pH and soil moisture content. The bioavailability of the test compound, and therefore the toxicity observed, is influenced by these soil properties. This means that results from different test soils cannot be compared directly. As far as possible, toxicity tests should be conducted in conditions (as regards the nature of the soil, its organic content and any other parameter that could influence the bioavailability of the substance) where the test substance is bioavailable to the tests organism(s). However, if possible data should be normalized using relationships that describe the bioavailability of chemicals in soils. Results are converted to a standard soil, which is defined as a soil with an organic matter content of 3.4% (see Section 2.3.4). For non-ionic organic compounds it is assumed that bioavailability is determined by the organic matter content only. NOECs and L(E)C50s are corrected according to the formula :

$$NOEC\ or\ L(E)C_{50(standard)} = NOEC\ or\ L(E)C_{50(\exp)} \cdot \frac{Fom_{soil(standard)}}{Fom_{soil(\exp)}} \qquad (71)$$

Explanation of symbols

NOEC or $L(E)C50_{exp}$	NOEC or L(E)C50 in experiment	$[mg \cdot kg^{-1}]$	
$Fom_{soil(standard)}$	fraction organic matter in standard soil	$[kg \cdot kg^{-1}]$	Table 5
$Fom_{soil(exp)}$	fraction organic matter in experimental soil	$[kg \cdot kg^{-1}]$	
NOEC or $L(E)C50_{standard}$	NOEC or L(E)C50 in standard soil	$[mg \cdot kg^{-1}]$	

It should be noted that this recommended normalisation is only appropriate when it can be assumed that the binding behaviour of a non-ionic organic substance in question is predominantly driven by its $logK_{ow}$, and that organisms are exposed predominantly *via* pore water.

Three situations can be distinguished for deriving a $PNEC_{soil}$:

- when no toxicity data are available for soil organisms, the equilibrium partitioning method is applied to identify a potential risk to soil organisms. This method is regarded as a "screening approach" and is explained in Section 3.6.2.1 (see also Section 3.5.2 sediment);
- when toxicity data are available for a producer, a consumer and/or a decomposer the $PNEC_{soil}$ is calculated using assessment factors as presented in Section 3.6.2.2;
- when only one test result with soil dwelling organisms is available the risk assessment is performed both on the basis of this result using assessment factors and on the basis of the equilibrium partition method. From both $PEC_{soil}/PNEC_{soil}$ ratios the highest one is chosen for the risk characterisation.

3.6.2.1 Calculation of PNEC using the equilibrium partitioning method

The equilibrium partitioning method may not be suitable for lipophilic compounds or substances with a specific mode of action nor for species that are exposed primarily through food (Van Gestel, 1992). Furthermore, this approach does not consider the effects on soil organisms of chemicals that are adsorbed to soil particles and taken up by ingestion.

The $PNEC_{soil}$ is calculated as follows:

$$PNEC_{soil} = \frac{K_{soil-water}}{RHO_{soil}} \cdot PNEC_{water} \cdot 1000 \qquad (72)$$

Explanation of symbols

$PNEC_{water}$	Predicted No Effect Concentration in water	$[mg \cdot l^{-1}]$	
RHO_{soil}	bulk density of wet soil	$[kg \cdot m^{-3}]$	eq. (18)
$K_{soil-water}$	partition coefficient soil water	$[m^3 \cdot m^{-3}]$	eq. (24)
$PNEC_{soil}$	Predicted No Effect Concentration in soil	$[mg \cdot kg^{-1}]$	

The applicability of the equilibrium partitioning method has been evaluated less for soil than for sediment-dwelling organisms. Van Gestel and Ma (1993) have shown the model to be valid for short-term toxicity of several chlorophenols, chlorobenzenes and chloroanilines to earthworms. In order to take uptake by soil ingestion into account the same approach is used as for the derivation of the $PNEC_{sediment}$. Thus, the $PEC_{soil}/PNEC_{soil}$ ratio is increased by a factor of 10 for compounds with a log Kow > 5 (or for compounds with a corresponding adsorption or binding behaviour, e.g. ionisable substances).

In principle, toxicity data for aquatic organisms cannot replace data for soil dwelling organisms. This is because the effects on aquatic species can only be considered as effects on soil organisms that are exposed exclusively to the soil pore water of the soil (Samsøe-Petersen and Pedersen, 1994). Therefore, if the $PEC_{soil}/PNEC_{soil}$ ratio that is calculated using the equilibrium partitioning method is greater than 1, tests with soil organisms should be considered as an essential requirement for a refined effects assessment.

3.6.2.2 Calculation of PNEC using assessment factors

The same assessment factors used for the aquatic compartment (see **Table 16**) are applied to the terrestrial compartment (see **Table 20**). The size of the assessment factor therefore again depends on the type of data that are available i.e. short-term or long-term toxicity test, the number of trophic levels tested and the general uncertainties in predicting ecosystem effects from laboratory data. The assessment factors suggested for the soil compartment are not based on comprehensive experience. As already stated information from tests with soil organisms will only be available for some compounds. Furthermore, in most cases this information will be from short-term tests with earthworms. This means that a deeper understanding of the difference between short- and long-term toxicity for several taxonomic groups and the difference between laboratory and field tests is needed. The choice of taxonomic groups for which toxicity data are necessary (conform the base-set of algae, Daphnia and fish for the aquatic environment), is also a point of discussion. A dataset comprising of toxicity data for primary producers, consumers and decomposers is preferred. However, an internationally accepted set of standardised

ecotoxicological tests for hazard assessment of chemicals for the soil compartment is not currently available.

Reference can be made to Section 6.3.4 and an OECD project in which a testing strategy for terrestrial ecosystems is being developed (Léon and Van Gestel, 1994). In summary, the assessment factors proposed in **Table 20** must be regarded as indicative. As more information on the sensitivity of soil organisms becomes available these factors may have to be revised.

Table 20 Assessment factors for derivation of $PNEC_{soil}$

Information available	Assessment factor
L(E)C50 short-term toxicity test(s) (e.g. plants, earthworms, or microorganisms)	1000
NOEC for one long-term toxicity test (e.g. plants)	100
NOEC for additional long-term toxicity tests of two trophic levels	50
NOEC for additional long-term toxicity tests for three species of three trophic levels	10
Species sensitivity distribution (SSD method)	5 – 1, to be fully justified on a case-by-case basis (cf. main text)
Field data/data of model ecosystems	case-by-case

A $PNEC_{soil}$ is calculated on the basis of the lowest determined effect concentration. If results from short-term tests with a producer, a consumer and/or a decomposer are available, the result is divided by a factor of 1000 to calculate the $PNEC_{soil}$. If only one terrestrial test result is available (earthworms or plants), the risk assessment should be performed both of this test result and on the basis of the outcome of the aquatic toxicity data to provide an indication of the risk. As a matter of precaution, the larger $PEC_{soil}/PNEC_{soil}$ ratio determines which further actions should be taken in the framework of the further testing strategy. If additional soil test results are available the assessment factors given in **Table 20** should be applied.

3.6.2.3 Calculation of PNEC using statistical extrapolation techniques

Calculation of a $PNEC_{soil}$ using statistical extrapolation techniques can be considered when sufficient data are available (see Section 3.3.1.2. for minumum requirements). For comparable data on the same end-point and species, by default the geometric mean should be used as the input value for the calculation of the species sensitivity distribution. When results are available from tests using different soils and it is likely that the soil characteristics have influence on the results, the effect data should be normalised before further processing. If not possible, the lowest NOEC per end-point and species should be used. Data on microbial mediated processes and single species tests should be considered separately due to fundamental differences between these tests (functional *vs.* structural test, multi-species *vs.* single species, adapted indigenous microbe community *vs.* laboratory test species, variability of test design and different endpoints, etc.). The results should be compared and evaluated on a case-by-case basis in deciding on a final PNEC for the soil compartment.

The approach of statistical extrapolation is still under debate and needs further validation.

3.7 EFFECTS ASSESSMENT FOR THE AIR COMPARTMENT

For the risk assessment of the air compartment biotic and abiotic effects are considered.

3.7.1 Biotic effects

The methodology used for effects assessment (and therefore the risk characterisation) of chemicals in water and soil cannot be applied yet in the same manner to the atmosphere. Methods for the determination of effects of chemicals on species arising from atmospheric contamination have not yet been fully developed, except for inhalation studies with mammals.

It is evident that the quantitative characterisation of risk by comparison of the PEC_{air} to $PNEC_{air}$ is not possible at the moment: only a qualitative assessment for air is feasible.

For the air compartment toxicological data on animal species other than mammals are usually not or only scarcely available. For volatile compounds acute or short-term inhalation tests may be present. On the basis of these data there may be indications of adverse effects. Short-term LC50 data can be used for a coarse estimation of the risk a chemical poses for animals. However, in most cases, it is unlikely that the atmospheric concentration of a chemical will be high enough to cause short-term toxic effects in the environment, so data on long-term or chronic toxicity should be considered. For example, a chemical may be dangerous for the atmospheric environment at a low concentration, if it is classified as R 48 ("Danger of serious damage to health by prolonged exposure"). Also mutagenic effects and toxic effects on reproduction by a chemical indicate a toxic potential for terrestrial vertebrates.

Fumigation tests on invertebrates are usually not available. For some existing substances and biocides investigations on the toxicity to honey bees (*Apis mellifera*), which are conducted according to guidelines for the testing of plant protection agents, may be available. In these tests, it is sometimes difficult to determine the effective concentration and therefore a $PNEC_{air}$ cannot be derived.

Concerning the toxicity for plants, data from tests where a chemical is applied directly via air (gaseous or deposited) are normally scarce. When toxicity data are available or information is available that plants might be affected this information must be carefully screened and if necessary further plant toxicity testing can be requested. When no specific information on toxicity to plants is available for the substance and considerable air emissions and exposure are expected the information on related compounds (e.g. toxicity, phys.chem. properties) should be screened and a decision should be made whether there is reason for concern and whether actual plant testing should be considered.

Some experience has been obtained over the last years on existing substances for which actual plant testing has been requested and performed (e.g. Risk assessment reports on tetrachloroethylene and dibutylphthalate, ECB, 2001). The test protocols have been developed on a case-by-case basis and varied from relatively simple laboratory test designs that can be considered as screening tests, to very extensive long-term open-top chambers with a large variety of species. Further discussion is needed before these test designs can be standardised and inserted in a more rigid testing strategy for plants.

How the results of the available toxicity test should be used in the actual setting of a PNEC for plants has yet to be decided on a case-by-case basis. Like with the effects assessments for the

other compartments it is expected that an assessment factor be applied to the available effects data. The selection of this factor should take into account factors such as:

- the type of tests that have been performed;
- the duration of these tests;
- the variety of species tested;
- the type and severity of the effects observed.

3.7.2 Abiotic effects

For the evaluation of an atmospheric risk, the following abiotic effects of a chemical on the atmosphere have to be considered:

- global warming;
- ozone depletion in the stratosphere;
- ozone formation in the troposphere;
- acidification.

If for a chemical there are indications that one or several of these effects occur, expert knowledge should be consulted. A first quantitative approach is described in De Leeuw (1993):

Global warming

The impact of a substance on global warming depends on its IR absorption characteristics and its atmospheric lifetime. A potential greenhouse gas shows absorption bands in the so-called atmospheric window (800-1,200 nm).

Stratospheric ozone

A substance may have an effect on stratospheric ozone if;

- the atmospheric lifetime is long enough to allow for transport to the stratosphere, and;
- it contains one or more Cl, Br or F substituents.

In general, ozone depletion potential values approach zero for molecules with atmospheric lifetimes less than one year.

Tropospheric ozone

The generation of tropospheric ozone depends on a number of factors:

- the reactivity of the substance and the degradation pathway;
- the meteorological conditions. The highest ozone concentrations are expected at high temperatures, high levels of solar radiation and low wind speeds;
- the concentration of other air pollutants. The concentration of nitrogen oxides has to exceed several ppb.

Highly reactive compounds (e.g. xylene, olefins or aldehydes) contribute significantly to the ozone peak values. Species with a low reactivity (e.g. CO, methane) are important for ozone formation in the free troposphere and therefore for the long-term ozone concentrations. However, all studies showed significant variability in the tropospheric ozone building potential values assigned to each organic component. It has to be concluded that at present there is no

procedure available to estimate the effect on tropospheric ozone if only the basic characteristics of a substance are known.

Acidification

During the oxidation of substances containing Cl, F, N or S substituents, acidifying components (e.g. HCl, HF, NO_2 and HNO_3, SO_2 and H_2SO_4) may be formed. After deposition, these oxidation products will lead to acidification of the receiving soil or surface water.

3.8 ASSESSMENT OF SECONDARY POISONING

3.8.1 Introduction

Bioconcentration and bioaccumulation may be of concern for lipophilic organic chemicals and some metal compounds as both direct and indirect toxic effects may be observed upon long-term exposure. For metals guidance is given in Appendix VIII. Bioconcentration is defined as the net result of the uptake, distribution and elimination of a substance in an organism due to water-borne exposure, whereas bioaccumulation includes all routes, i.e. air, water, soil and food. Biomagnification is defined as accumulation and transfer of chemicals via the food chain, resulting in an increase of the internal concentration in organisms at higher levels in the trophic chain. Secondary poisoning is concerned with toxic effects in the higher members of the food chain, either living in the aquatic or terrestrial environment, which result from ingestion of organisms from lower trophic levels that contain accumulated substances.

For many hydrophobic chemicals, accumulation through the food chain follows many different pathways along different trophic levels. A good risk estimation of this complex process is hampered when only limited data from laboratory studies are available. One way to assess a chemicals risk for bioaccumulation in aquatic species is to measure the Bioconcentration Factor (BCF). The static bioconcentration factor is the ratio between the concentration in the organism and the concentration in water in a steady-state (sometimes also called equilibrium) situation. When uptake and depuration kinetics are measured, the dynamic bioconcentration factor can be calculated from the quotient of the uptake and depuration rate constants:

$$BCF_{fish} = \frac{C_{fish}}{C_{water}} \quad or \quad \frac{k_1}{k_2} \tag{73}$$

Explanation of symbols

C_{fish}	concentration in fish	$[mg \cdot kg^{-1}]$
C_{water}	concentration in water	$[mg \cdot l^{-1}]$
k_1	uptake rate constant from water	$[l \cdot kg^{-1} \cdot d^{-1}]$
k_2	elimination rate constant	$[d^{-1}]$
BCF_{fish}	bioconcentration factor	$[l \cdot kg^{-1}]$

For new and existing substances, the assessment of these processes is revised as more information becomes available on toxicological and ecotoxicological effects and exposure. At the base-set level the available physico-chemical and (eco)toxicological information can be used to decide whether or not there are indications for a potential for bioaccumulation and/or indirect

effects. This estimation is used as a first step in the testing strategy for bioaccumulation and secondary poisoning as will be explained in Section 3.8.3. For the terrestrial ecosystem a similar strategy is used which is described in Section 3.8.3.7.

3.8.2 Indication of bioaccumulation potential

The simplest way to estimate the potential of a substance to bioaccumulate in aquatic species is by experimental measurement of the BCF. Determination of the BCF alone, however, only gives a partial picture of the potential of bioaccumulation, and additional data on uptake and depuration kinetics, metabolism, organ specific accumulation and the level of bound residues may also be required. Such data will rarely be available and the potential for bioaccumulation will usually need to be determined using simple physico-chemical and structural evidence (OECD, 2001c).

The most important and widely accepted indication of bioaccumulation potential is a high value of the n-octanol/water partition coefficient. In addition, if a substance belongs to a class of chemicals, which are known to accumulate in living organisms, it may have a potential to bioaccumulate. However, some properties of a substance may preclude high accumulation levels even though the substance has a high log Kow or has a structural similarity to other substances likely to bioaccumulate. Alternatively there are properties, which may indicate a higher bioaccumulation potential than that suggested by a substance's low log Kow value. A survey of these factors is given below.

n-Octanol/water partition coefficient

At the base-set level, the potential for bioaccumulation can be estimated from the value of the n-octanol/water partition coefficient, log Kow. If this value cannot be determined experimentally, it may be calculated from the chemical structure.

It is accepted that values of log Kow greater than or equal to 3 indicate that the substance may bioaccumulate. For certain types of chemicals, e.g. surface-active agents and those which ionise in water, log Kow values may not be suitable for calculation of a BCF value. There are, however, a number of factors that are not taken into consideration when BCF is estimated only on the basis of log Kow values. These are:

- phenomena of active transport;
- metabolism in organisms and the accumulation potential of any metabolites;
- affinity due to specific interactions with tissue components;
- special structural properties (e.g. amphiphilic substances or dissociating substances that may lead to multiple equilibrium processes);
- uptake and depuration kinetics (leading for instance to a remaining concentration plateau in the organism after depuration).

n-Octanol only simulates the lipid fraction in organisms and therefore does not simulate other possibilities for storage and accumulation of substances and their metabolites in living organisms.

Adsorption

Adsorption onto biological surfaces, such as gills or skin, may also lead to bioaccumulation and an uptake via the food chain. Hence, high adsorptive properties may indicate a potential for both

bioaccumulation and biomagnification. For certain chemicals, for which the octanol/water partition coefficient cannot be measured properly, a high adsorptive capacity (of which log Kp > 3 may be an indication) can be additional evidence of bioaccumulation potential.

Hydrolysis

The effect of hydrolysis may be a significant factor for substances discharged mainly to the aquatic environment: the concentration of a substance in water is reduced by hydrolysis so the extent of bioconcentration in aquatic organisms would also be reduced. Where the half-life, at environmentally relevant pH values (4-9) and temperature, is less than 12 hours, it can be assumed that the rate of hydrolysis is greater than that for uptake by the exposed organisms. Hence, the likelihood of bioaccumulation is greatly reduced. In these cases, it may sometimes be appropriate to perform a BCF test on the hydrolysis products, if identified, instead of the parent substance. However, it should be noted that, in most cases hydrolysis products are more hydrophilic and as a consequence will have a lower potential for bioaccumulation.

Degradation

Both biotic and abiotic degradation may lead to relatively low concentrations of a substance in the aquatic environment and thus to low concentrations in aquatic organisms. However, the uptake rate may still be greater than the rate of the degradation processes, leading to high BCF values even for readily biodegradable substances. Therefore ready biodegradability does not preclude a bioaccumulation potential, but for most substances concentrations will be low in aquatic organisms.

At the base-set level, only scarce information on the kinetics of degradation is available. For new substances even at higher tonnages, a request for such information would need to be justified; it can be requested only on a case-by-case basis at level 2. For existing substances information on degradation kinetics may be available.

If persistent metabolites are formed in substantial amounts the bioaccumulation potential of these substances should also be assessed. However, for most substances information will be scarce. From experiments with mammals information may be obtained on the formation of possible metabolites, although extrapolation of results should be treated with care.

Molecular mass

Certain classes of substances with a molecular mass greater than 700 are not readily taken up by fish, because of possible steric hindrance at passage of gill membranes or cell membranes of respiratory organs. These substances are unlikely to bioaccumulate significantly (regardless of the log Kow-value).

Summary of indications of bioaccumulation potential

Taking the factors mentioned above into account will indicate whether or not there is potential for bioaccumulation. In summary: if, at base-set level, a substance:

- has a log Kow ≥ 3; or;
- is highly adsorptive; or;
- belongs to a class of substances known to have a potential to accumulate in living organisms; or;
- there are indications from structural features;
- and there is no mitigating property such as hydrolysis (half-life less than 12 hours);

there is an indication of bioaccumulation potential.

Reference is made to the OECD guidelines and to the guidance document on environmental hazard classification (OECD, 2001c) in relation to interpretation of bioaccumulation studies and measurements of logKow. The test guidelines also contain information on the suitability of the various log Kow determination methods depending on the type of substance concerned.

3.8.3 Effects assessment for bioaccumulation and secondary poisoning

3.8.3.1 General approach

The assessment of the potential impact of substances on top predators is based on the accumulation of hydrophobic chemicals through the food chains which may follow many different pathways along different trophic levels. This accumulation may result in toxic concentrations in predatory birds or mammals ingesting biota containing the chemical. This effect is called secondary poisoning and should in principle be assessed by comparing the measured or estimated concentrations in the tissues and organs of the top predators with the no-effect concentrations for these predators expressed as the internal dose. In practice, however, data on internal concentrations in wildlife animals are hardly ever available and most no-effect levels are expressed in term of concentrations of the food that the organisms consume (i.e. in $mg \cdot kg^{-1}$ food). Therefore, the actual assessment (see below) is normally based on a comparison of the (predicted) concentration in the food of the top predator and the (predicted) no-effect concentration which is based on studies with laboratory animals. A distinction is made between the methodology used to assess the effects of substances whose effects can be related directly to bioconcentration (direct uptake via water) and those where also indirect uptake via the food may contribute significantly to the bioaccumulation. Bioaccumulation of metallic species is not considered explicitly in this section.

For substances with a log Kow < 4.5 the primary uptake route is direct uptake from the water phase. In the absence of data on other uptake routes, it is assumed that the direct uptake accounts for 100% of the intake. For substances with a log Kow ≥ 4.5, other uptake routes such as intake of contaminated food or sediment may become increasingly important. Especially the uptake through the food chains eventually leading to secondary poisoning should be considered and a strategy for the assessment of secondary poisoning has been developed. This strategy takes account of the $PEC_{aquatic}$, the direct uptake and resulting concentration in food of aquatic organisms and the mammalian and avian toxicity of the chemical. On this basis, possible effects are estimated on birds and mammals in the environment via uptake through the food-chain water → aquatic organisms → fish → fish-eating mammal or fish-eating bird (Romijn et al., 1993). Due to the lack of experience with this approach the assessment is considered as provisional.

For some chemicals results from field measurements are available. Although interpretation is often difficult, these results can be used to support the assessment of risks due to secondary poisoning (Ma, 1994).

The first step in the assessment strategy is to consider whether there are indications for bioaccumulation potential. These indications have been discussed in the previous section. Subsequently, it is necessary to consider whether the substance has a potential to cause toxic effects if accumulated in higher organisms. This assessment is based on classifications on the basis of mammalian toxicity data, i.e. the classification Very Toxic (T+) or Toxic (T) or harmful (Xn) with at least one of the risk phrases R48 "Danger of serious damage to health by prolonged exposure", R60 "May impair fertility", R61 "May cause harm to the unborn child", R62 "Possible risk of impaired fertility", R63 "Possible risk of harm to the unborn child", R64 "May cause harm to breastfed babies". Here it is assumed that the available mammalian toxicity data can give an indication on the possible risks of the chemical to higher organisms in the environment.

The current, either qualitative or quantitative, approach in the human health risk assessment for genotoxic carcinogens is not practicable in the environmental part. Tumor incidence rates for a genotoxic carcinogen and subsequent cancer risks are related to individual risks in man and it is in most cases difficult to link those effects to populations. Endangoured species might be an exception, particularly those characterized by long-life-cycles where individuals may need to be protected to support survival of the species. It is not unlikely, however, that the conservative approach followed in the risk assessment for man indirectly exposed via the environment for genotoxic substances, will also be protective for individual top predators.

If a substance is classified accordingly or if there are other indications (e.g. endocrine disruption), an assessment of secondary poisoning is performed.

A schematic view of the assessment scheme for the exposure route water → aquatic organisms → fish → fish-eating mammal or fish-eating bird described above is given in **Figure 14**.

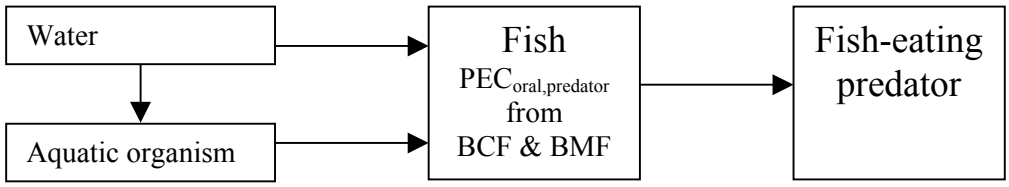

Figure 14. Assessment of secondary poisoning

No specific assessment of the risk to fish as a result of the combined intake of contaminants from water and contaminated food (aquatic organism) is considered necessary as this is assumed to be covered by the aquatic risk assessment and the risk assessment for secondary poisoning of fish-eating predators.

The risk to the fish-eating predators (mammals and/or birds) is calculated as the ratio between the concentration in their food ($PECoral_{predator}$) and the no-effect-concentration for oral intake ($PNEC_{oral}$). The concentration in fish is a result of uptake from the aqueous phase and intake of contaminated food (aquatic organisms). Thus, $PECoral_{predator}$ is calculated from the bioconcentration factor (BCF) and a biomagnification factor (BMF). Note that $PECoral_{predator}$ could also be calculated for other relevant species that are part of the food of predators.

The details of the individual assessment steps are described in the following sections.

3.8.3.2 Calculation of BCF from log Kow

If measured BCF values are not available, the BCF for fish can be predicted from the relationship between Kow and BCF. Various methods are available to calculate Kow. Often a large variation is found in the Kow values of a chemical by using different methods. Therefore the Kow-value must have been evaluated by an expert (see also Chapter 4 on the use of QSARs). For substances with a log Kow of 2-6 the following linear relationship can be used as developed by Veith et al. (1979).

$$\log BCF_{fish} = 0.85 \cdot \log Kow - 0.70 \quad (74)$$

Explanation of symbols

Kow	octanol-water partition coefficient	[-]
BCF_{fish}	bioconcentration factor for fish on wet weight basis	[l · $kg_{wet\ fish}$]

For substances with a log Kow higher than 6 a parabolic equation can be used.

$$\log BCF_{fish} = -0.20 \cdot logKow^2 + 2.74 \cdot \log Kow - 4.72 \quad (75)$$

Explanation of symbols

Kow	octanol-water partition coefficient	[-]
BCF_{fish}	bioconcentration factor for fish on wet weight basis	[l · $kg_{wet\ fish}$]

It should be noted that due to experimental difficulties in determining BCF values for such substances this mathematical relationship has a higher degree of uncertainty than the linear one. Both relationships apply to compounds with a MW less than 700. For a discussion on both relationships see Chapter 4 (Use of QSARs).

3.8.3.3 Experimentally derived BCF

For existing substances an experimentally derived BCF may be present. For new substances a BCF test is mandatory at level 1. In most cases preference should be given to experimentally determined BCF values, especially if the test is conducted according to EU Annex V C.13 and OECD guideline 305 (OECD, 1996). The following parameters may be of importance when considering the results of testing:

- BCF (bioconcentration factor);
- CT50 (clearance time, elimination or depuration expressed as half-life);
- metabolism/ transformation;
- organ-specific accumulation (reversible/ irreversible);
- incomplete elimination (bound residues);
- substance bioavailability.

Recent work has shown that tests with substances with a high log Kow value result in high bioaccumulation factors if the chemical is carefully tested within the limit of its water solubility,

i.e. without enhancement of solubility by the use of solubilisers. Also, the test duration is very important because for highly hydrophobic chemicals it may take a very long time before a true steady-state situation between water and organism has been reached. In addition, such lipophilic substances may be adsorbed onto biological surfaces such as gills, skin etc. which may lead to toxic effects in higher organisms after biomagnification.

For a more detailed guidance on interpretation of bioaccumulation test data, the OECD guidance document on environmental hazard classification (OECD, 2001c) may be consulted.

3.8.3.4 Calculation of a predicted environmental concentration in food

The concentration of contaminant in food (fish) of fish-eating predators ($PECoral_{predator}$) is calculated from the PEC for surface water, the measured or estimated BCF for fish and the biomagnification factor (BMF):

$$PEC_{oral,predator} = PEC_{water} \cdot BCF_{fish} \cdot BMF \qquad (76)$$

Explanation of symbols

$PECoral_{predator}$	Predicted Environmental Concentration in food	$[mg \cdot kg_{wet\ fish}^{-1}]$
PEC_{water}	Predicted Environmental Concentration in water	$[mg \cdot l^{-1}]$
BCF_{fish}	bioconcentration factor for fish on wet weight basis	$[l \cdot kg_{wet\ fish}^{-1}]$
BMF	biomagnification factor in fish	[-]

Table 21

The BMF is defined as the relative concentration in a predatory animal compared to the concentration in its prey (BMF = Cpredator/Cprey). The concentrations used to derive and report BMF values should, where possible, be lipid normalised.

An appropriate PEC_{water} reflecting the foraging area of fish-eating mammals and birds should be used for the estimate. The foraging area will of course differ between different predators, which makes it difficult to decide on an appropriate scale. For example use of PEClocal may lead to an overestimation of the risk as fish-eating birds or mammals do also forage on fish from other sites than the area around the point of discharge. Also, biodegradation in surface water is not taken into account using PEClocal. However, using PECregional may have the opposite effect, as there may be large areas in the 200 · 200 km region with higher concentrations. It has therefore been decided that a scenario where 50% of the diet comes from a local area (represented by the annual average PEClocal) and 50% of the diet comes from a regional area (represented by the annual average PECregional) is the most appropriate for the assessment.

The biomagnification factor (BMF) should ideally be based on measured data. However, the availability of such data is at present very limited and therefore, the default values given in **Table 21** should be used. By establishing these factors it is assumed that a relationship exists between the BMF, the BCF and the log Kow (for further explanation, see Section 4.3.3 on marine risk assessment). When measured BCF values are available, these should form the basis for deciding on the size of the BMF.

Table 21 Default BMF values for organic substances

log Kow of substance	BCF (fish)	BMF
<4.5	< 2,000	1
4.5 - <5	2,000-5,000	2
5 – 8	> 5,000	10
>8 – 9	2,000-5,000	3
>9	< 2,000	1

3.8.3.5 Calculation of the predicted no-effect concentration (PNECoral)

Only toxicity studies reporting on dietary and oral exposure are relevant as the pathway for secondary poisoning is referring exclusively to the uptake through the food chain. Secondary poisoning effects on bird and mammal populations rarely become manifest in short-term studies. Therefore, results from long-term studies are strongly preferred, such as NOECs for mortality, reproduction or growth. If no adequate toxicity data for mammals or birds are available, an assessment of secondary poisoning cannot be made.

For new substances, the results of mammalian repeated-dose toxicity tests are used to assess secondary poisoning effects. For existing substances and biocides, toxicity data for birds (e.g. OECD test 205 (1984h) (LC50, 5-day acute avian dietary study) or OECD test 206 (1984i) (chronic)) may also be present. Extrapolation from such test results gives a predicted no-effect concentration in food (PNECoral) that should be protective to other mammalian and avian species.

Acute lethal doses LD50 (rat, bird) are not acceptable for extrapolation to chronic toxicity, as these are not dietary tests. Acute effect concentrations (e.g. OECD 205 (1984h)) for birds are acceptable for extrapolation. The results of the available mammalian or avian tests may be expressed as a concentration in the food ($mg \cdot kg_{food}^{-1}$) or a dose ($mg \cdot kg$ body $weight \cdot day^{-1}$) causing no effect. For the assessment of secondary poisoning, the results always have to be expressed as the concentration in food. In case toxicity data are given as NOAEL only, these NOAELs can be converted to NOECs with the following two formulae:

$$NOEC_{bird} = NOAEL_{bird} \cdot CONV_{bird} \tag{77}$$

$$NOEC_{mammal,food\_chr} = NOAEL_{mammal,oral\_chr} \cdot CONV_{mammal} \tag{78}$$

Explanation of symbols

$NOEC_{bird}$	NOEC for birds	$(kg \cdot kg_{food}^{-1})$	
$NOEC_{mammal,\ food\ chr}$	NOEC for mammals	$(kg \cdot kg_{food}^{-1})$	
$NOAEL_{bird}$	NOAEL for birds	$(kg \cdot kg\ bw \cdot d^{-1})$	
$NOAEL_{mammal,\ oral\ chr}$	NOAEL for mammals	$(kg \cdot kg\ bw \cdot d^{-1})$	
$CONV_{bird}$	conversion factor from NOAEL to NOEC	$(kg\ bw \cdot d \cdot kg_{food}^{-1})$	Table 22
$CONV_{mammal}$	conversion factor from NOAEL to NOEC	$(kg\ bw \cdot d \cdot kg_{food}^{-1})$	Table 22

Conversion factors for laboratory animals are presented in **Table 22**.

Table 22 Conversion factors from NOAEL to NOEC for several mammalian and one bird species

Species	Conversion factor (bw/dfi)
Canis domesticus	40
Macaca sp.	20
Microtus spp.	8.3
Mus musculus	8.3
Oryctolagus cuniculus	33.3
Rattus norvegicus (> 6 weeks)	20
Rattus norvegicus (≤ 6 weeks)	10
Gallus domesticus	8

* bw = body weight (g); dfi: daily food intake (g/day)

NOECs converted from NOAELs have the same priority as direct NOECs.

The PNECoral is ultimately derived from the toxicity data (food basis) applying an assessment factor. In formula:

$$PNEC_{oral} = \frac{TOX_{oral}}{AF_{oral}} \tag{79}$$

Explanation of symbols

PNECoral	PNEC for secondary poisoning of birds and mammals	[in $kg \cdot kg_{food}^{-1}$]	
AForal	assessment factor applied in extrapolation of PNEC	[-]	Table 23
TOXoral	either $LC50_{bird}$, $NOEC_{bird}$ or $NOEC_{mammal, food, chr}$	[in $kg \cdot kg_{food}^{-1}$]	

The assessment factor (AForal) takes into account interspecies variation, acute/subchronic to chronic extrapolation and laboratory data to field impact extrapolation. Some specific considerations need to be made for the use of the assessment factor for predators.

CCME (1998) contains wildlife data on body weight and daily food ingestion rates for 27 bird and 10 mammalian species. In addition, Schudoma et al. (1999) derived the mean body weight and daily food intake for the otter. The currently available set on wildlife bw/dfi ratios ranges from 1.1 to 9 for birds and from 3.9 to 10 for mammalian species. Comparison of these wildlife conversion factors with the values given in **Table 22** for laboratory species (8.3 – 40) shows that the wildlife species often have a lower bw/dfi ratio than laboratory animals. The difference can be up to a factor 8 for birds and 10 for mammals. This difference is in theory accounted for in the use of the interspecies variation factor that is part of the standard assessment factor. The interspecies variation, however, should comprise more than just the bw/dfi differences between species, e.g. the differences in intrinsic sensitivity. The protective value of the "normal" interspecies variation factor may therefore be questionable in case of predators. On top of that, many predator species are characterised by typical metabolic stages in their life-cycle that could make them extra sensitive to contaminants in comparison with laboratory animals (e.g.

hibernation or migration). Similar to the bw/dfi differences, also this aspect goes beyond the "normal" interspecies variation.

The AForal should compensate for the above-mentioned specific aspects in the effects assessment of predators. A factor of 30, accounting for both interspecies variation and lab-to-field extrapolation, is considered to be appropriate for this purpose. Aditionally, acute/subchronic to chronic extrapolation needs to be taken into account. The resulting assessment factors are given in **Table 23**.

Table 23 Assessment factors for extrapolation of mammalian and bird toxicity data

TOXoral	Duration of test	AForal
$LC50_{bird}$	5 days	3,000
$NOEC_{bird}$	chronic	30
$NOEC_{mammal,\ food,chr}$	28 days 90 days chronic	300 90 30

If a NOEC for both birds and mammals is given, the lower of the resulting PNECs is used in the risk assessment.

3.8.3.6 Assessment of secondary poisoning via the aquatic food chain

It should be recognised that the schematic aquatic food chain water → aquatic organism → fish → fish-eating bird or mammal is a very simplistic scenario as well as the assessment of risks for secondary poisoning based on it. Any other information that may improve the input data or the assessment should therefore be considered as well. For substances where this assessment leads to the conclusion that there is a risk of secondary poisoning, it may be considered to conduct additional laboratory tests (e.g. tests of bioaccumulation in fish or feeding studies with laboratory mammals or birds) in order to obtain better data.

The simplified food chain is only one example of a secondary poisoning pathway. Safe levels for fish-eating animals do not exclude risks for other birds or mammals feeding on other aquatic organisms (e.g. mussels and worms). Therefore it is emphasised that the proposed methodology gives only an indication that secondary poisoning is a critical process in the aquatic risk characterisation of a chemical.

For a more detailed analysis of secondary poisoning, several factors have to be taken into account (US EPA, 1993; Jongbloed et al., 1994):

- differences in metabolic rates between animals in the laboratory and animals in the field;
- normal versus extreme environmental conditions: differences in metabolic rate under normal field conditions and more extreme ones, e.g. breeding period, migration, winter;
- differences in caloric content of different types of food: cereals versus fish, worms or mussels. As the caloric content of fish is lower than cereals birds or mammals in the field must consume more fish compared to cereals for the same amount of energy needed leading to a higher body burden of the pollutant;
- pollutant assimilation efficiency: differences in bioavailability in test animals (surface application of a test compound) and in the field (compound incorporated in food) and/or;

- relative sensitivity of animals for certain chemicals: differences in biotransformation of certain compounds between taxonomic groups of birds or mammals. The US EPA uses a species sensitivity factor (SSF) which ranges from 1 to 0.01.

Whether these factors should be used is still under debate.

3.8.3.7 Assessment of secondary poisoning via the terrestrial food chain

Biomagnification may also occur via the terrestrial food chain. A similar approach as for the aquatic route can be used here. The food-chain soil → earthworm → worm-eating birds or mammals is used as has been described by Romijn et al. (1994). The PNECoral is derived in the same way as for the aquatic route (see Section 3.8.3.5). Since birds and mammals consume worms with their gut contents and the gut of earthworms can contain substantial amounts of soil, the exposure of the predators may be affected by the amount of substance that is in this soil. The $PECoral_{predator}$ is calculated as:

$$PEC_{oral,\ predator} = C_{earthworm} \tag{80}$$

where $C_{earthworm}$ is the total concentration of the substance in the worm as a result of bioaccumulation in worm tissues and the adsorption of the substance to the soil present in the gut.

For PEC_{soil} the PEClocal is used in which with respect to sludge application the concentration is averaged over a period of 180 days (see Section 2.3.8.5). The same scenario is used as for the aquatic food chain (see Section 3.8.3.4): i.e. 50% of the diet comes from PEClocal and 50% from PECregional.

Gut loading of earthworms depends heavily on soil conditions and available food (lower when high quality food like dung is available). Reported values range from 2-20 % (kg dwt gut/kg wwt voided worm), 10% can therefore be taken as a reasonable value. The total concentration in a full worm can be calculated as the weighted average of the worm's tissues (through BCF and porewater) and gut contents (through soil concentration):

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} \cdot W_{earthworm} + C_{soil} \cdot W_{gut}}{W_{earthworm} + W_{gut}} \tag{81}$$

Explanation of symbols

$PECoral_{predator}$	Predicted Environmental Concentration in food	$[mg \cdot kg_{wet\ earthworm}^{-1}]$
$BCF_{earthworm}$	bioconcentration factor for earthworms on wet weight basis	$[L \cdot kg_{wet\ earthworm}^{-1}]$
$C_{earthworm}$	concentration in earthworm on wet weight basis	$[mg \cdot kg_{wet\ earthworm}^{-1}]$
$C_{porewater}$	concentration in porewater	$[mg \cdot L^{-1}]$
C_{soil}	concentration in soil	$[mg \cdot kg_{wwt}^{-1}]$
$W_{earthworm}$	weight of earthworm tissue	$[kg_{wwt\ tissue}]$
W_{gut}	weight of gut contents	$[kg_{wwt}]$

The weight of the gut contents can be rewritten using the fraction of gut contents in the total worm:

$$W_{gut} = W_{earthworm} \cdot F_{gut} \cdot CONV_{soil} \tag{82a}$$

where:

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid} \cdot RHO_{solid}} \tag{82b}$$

Explanation of symbols

$CONV_{soil}$	conversion factor for soil concentration wet-dry weight soil	$[kg_{wwt} \cdot kg_{dwt}^{-1}]$	
F_{solid}	volume fraction of solids in soil	$[m^3 \cdot m^{-3}]$	Table 5
F_{gut}	fraction of gut loading in worm	$kg_{dwt} \cdot kg_{wwt}^{-1}$	0.1
RHO_{soil}	bulk density of wet soil	$[kg_{wwt} \cdot m^{-3}]$	eq. (18)
RHO_{solid}	density of solid phase	$[kg_{dwt} \cdot m^{-3}]$	Table 5

Using this equation, the concentration in a full worm can be written as:

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} + C_{soil} \cdot F_{gut} \cdot CONV_{soil}}{1 + F_{gut} \cdot CONV_{soil}} \tag{82c}$$

When measured data on bioconcentration in worms is available the BCF factors can be inserted in the above equation. For most substances, however, these data will not be present and BCF will have to be estimated. For organic chemicals, the main route of uptake into earthworms will be via the interstitial water. Bioconcentration can be described as a hydrophobic partitioning between the pore water and the phases inside the organism and can be modelled according to the following equation as described by Jager (1998):

$$BCF_{earthworm} = \left(0.84 + 0.012K_{ow}\right) / RHO_{earthworm} \tag{82d}$$

where for $RHO_{earthworm}$ by default a value of 1 ($kg_{wwt} \cdot L^{-1}$) can be assumed.

Jager (1998) has demonstrated that this approach performed very well in describing uptake in experiment with earthworms kept in water. For soil exposure, the scatter is larger and the experimental BCFs are generally somewhat lower than the predictions by the model. The reasons for this discrepancy are unclear but may include experimental difficulties (a lack of equilibrium or purging method) or an underestimated sorption.[4]

[4] According to certain studies some soil ingesting organisms may accumulate chemical substances not only from the soil pore water but also directly (possibly by extraction in the digestive tract) from the fraction of the substance adsorbed onto soil particles. This may become important for strongly adsorbing chemicals, e.g. those with a logKow > 3. For these compounds the total uptake may be underestimated. In other studies however it has been shown that soil digesters virtually only bioaccumulate the substance via the pore water, i.e. bioconcentrate chemical substances from the soil pore water. At present the latter process can be modelled by use of the equilibrium partitioning theory (cf. also Section 3.5).

Earthworms are also able to take up chemicals from food and it has been hypothesized that this process may affect accumulation at log Kow>5 (Belfroid et al., 1995). The data collected by Jager (1998), however, do not indicate that this exposure route actually leads to higher body residues than expected on the basis of simple partitioning. Care must be taken in situations where the food of earthworms is specifically contaminated (e.g. in case of high concentrations in leaf litter) although reliable models to estimate this route are currently lacking.

The model was supported by data with neutral organic chemicals in soil within the range log Kow 3-8 and in water-only experiments from 1-6. An application range of 1-8 is advised and it is reasonable to assume that extrapolation to lower Kow values is possible. The model could also be used for chlorophenols when the fraction in the neutral form was at least 5% and when both sorption and BCF are derived from the Kow of the neutral species. The underlying data are however too limited to propose this approach in general for ionised chemicals.

4 ENVIRONMENTAL RISK ASSESSMENT – MARINE

4.1 INTRODUCTION

The extension of the existing risk assessment approaches to cover risks to the marine environment is a logical and important development in the establishment of a comprehensive risk assessment methodology. Both the Commission report on the operation of several pieces of legislation in the area of chemicals (COMMISSION, SEC (1998) 1986 final) as well as the OSPAR Hazardous Substances Strategy (OSPAR, 1998) recognise the need to extend the risk assessment framework and methodology as developed under Directive 93/67 and Regulation EC 1488/94. This section, therefore, seeks to lay down the principles and concepts that should drive an assessment of the impacts on the marine environment. In doing so, it also identifies the areas where a similar approach can be adopted to that described elsewhere within the TGD, as well as elaborating different methodologies where they are considered more appropriate.

The assessment approaches detailed within the TGD have been developed principally to address risks, which might arise from emissions to the terrestrial and/or limnic aquatic environment. These schemes can and must nevertheless act as a starting point for the development of a comprehensive approach to risk assessment of substances in the marine environment, although due recognition is given to the many differences both in technical detail and general approaches which may be necessary. It is not the intention of this section, therefore, to repeat technical descriptions or equations described elsewhere where the basic methodology for marine assessment do not differ significantly to that applied to the freshwater environment. Such technical detail will be appropriately referenced to ensure that clarity is maintained. Rather, the section will focus on new approaches, which are considered necessary to cover the unique features of the marine environment.

While the approaches to the assessment must conform to EC requirements for assessment under Directive 67/548, Regulation 793/93 and Directive 98/8, they must also recognise the objectives established by OSPAR policy. The approaches will be guided and implemented, therefore, in accordance with the EU policy under the above legislation as well as taking into account the OSPAR Strategy on Hazardous Substances. With respect to the OSPAR strategy the assessment should specifically contribute to the identification of the sources of release for a chemical and their relative significance in order to facilitate the eventual preparation of measures that substantially, effectively and proportionately reduce the exposure.

The basic principles of the assessment have been derived in accordance with the experience gathered by the procedure for chemicals in the frame of the original TGD (EC, 1996). In attempting to extend current risk assessment methodology to cover the marine environment, it is necessary to closely investigate the common concepts and protection goals of the available methods. Where common protection goals were identified, an examination of the appropriateness of the current methodologies to achieve them has been carried out. Modifications have been made where necessary to enhance relevance to the marine environment. Where environmental compartments were not adequately covered by the existing methodologies, new approaches have been elaborated based on a sound scientific understanding of the problems and taking account, where appropriate, of the precautionary principle.

The approaches of the original TGD for the inland environment and that required for assessment of the marine environment share a number of common principles and objectives. Each must attempt to address the concern for the potential impact of individual substances on the

environment by examining both the exposures resulting from discharges/releases of chemicals and the effects of such emissions on the structure and function of the ecosystem. In the TGD for the inland environment this is practically done by considering five environmental compartments, namely the aquatic ecosystem, the terrestrial ecosystem, top predators, the functioning of Sewage Treatment Plants (STP) and the atmosphere. The environmental compartments are assessed at the local and the regional spatial scale by comparing the **P**redicted **E**nvironmental **C**oncentration (**PEC**) with the **P**redicted **N**o **E**ffect **C**oncentration (**PNEC**) for the ecosystem using data from representative species at different trophic levels for the particular environmental compartment. Top predators are assessed by assuming an exposure through the food chain. The assessment addresses the functioning of the ecosystem as determined by the survival and well-being of all the species in the specific ecosystem. It is assumed that the protection of species protects ecosystem structure and hence the ecosystem function. It addresses the survival and well-being of species populations rather than an individual organism.

While this approach must clearly also apply to the marine environment, it must be recognised that the concepts and methodologies for the inland environment have largely been developed with the local and regional spatial scales in mind, rather than the potential for global impact. There are, therefore, additional concerns for the risk assessment of the marine environment, which may not be adequately addressed by the methodologies used for the inland environmental risk assessment. These are:

a. the concern that hazardous substances may accumulate in parts of the marine environment and that:
   (i) the effects of such accumulation are unpredictable in the long-term;
   (ii) that such accumulation would be practically difficult to reverse;

b. the concern that remote areas of the oceans should remain untouched by hazardous substances resulting from human activity, and that the intrinsic value of pristine environments should be protected.

Of these additional concerns (a) above may be seen as the main concern. This is characterised by a spatial and temporal scale not covered by the inland risk assessment approach. It is a concern that chemical substances which can be shown both to persist for long periods and bioaccumulate in biota, can give rise to toxic effects after a greater time and at a greater distance than chemicals without these properties. While this is also true for the freshwater environment, the additional concern in the marine environment is that once the chemical has entered the open seas, any cessation of emission will not necessarily result in a reduction in chemical concentration and hence any effects become difficult to reverse. Equally, because of the long-term exposures and long-life-cycle of many important marine species, effects may be difficult to detect at an early stage.

To meet these concerns, which principally relate to substances that are considered as Persistent, Bioaccumulative and Toxic (referred to as PBTs), or have other properties which give rise to a similar level of concern, an assessment approach will be detailed that will give special consideration to this new protection goal. In this context, the assessment of risk fulfils specifically the purpose of determining what are the sources, routes and pathways to the marine environment. This assessment will facilitate in the subsequent risk management decisions on which measures are the most effective in order to reduce the levels.

The structure of this section on marine risk assessment basically follows the structure of the inland environmental assessment. It starts with a section of exposure assessment where specific issues are highlighted relating to marine partitioning processes and marine degradation and

where a description is given on how the predicted environmental concentration (PEC) for the local and regional situation should be derived. In the next section on marine effects assessment the specific procedures for the derivation of predicted no-effect concentrations (PNECs) for the aquatic compartment and for sediment are described. This section also deals with the assessment of possible effects through secondary poisoning via the foodchain in the marine environment. The section ends with the section on PBT assessment that describes criteria for identification of persistent, bioaccumulative and toxic substances and includes testing strategies to obtain the necessary data for this identification. For the risk characterisation the reader is referred to Section 5.

4.2 MARINE EXPOSURE ASSESSMENT

4.2.1 Measured data

Guidance on the use of measured data in the environmental exposure assessment can be found in Section 2.2 of the TGD for the inland environment. This section covers the selection of adequate data, the allocation of these data to the regional or local scale and deals with the question whether measured or estimated data (or both) should be used in the risk characterisation phase.

4.2.2 Partition coefficients

The distribution of a substance in the environment can be predicted from partition coefficients, which describe the relative concentrations between environmental compartments at equilibrium. Specific information on the derivation of the partitioning processes between air-aerosol, air-water, and solids-water in the various compartments can be found in Section 2.3.5. This section only highlights some specific issues related to the marine environmental conditions.

Measured partition coefficients between water and a second compartment, if available, are usually derived from studies using non-saline water (freshwater or distilled/deionised water). In the absence of measured data, the relevant partition coefficients must be extrapolated from the primary data listed in Section 2.3.2. However, the techniques that allow such an extrapolation are also largely based on freshwater data sets. Therefore, to assess the distribution of chemicals in the marine environment, it is necessary to consider the extent to which partition coefficients may differ between seawater and freshwater.

The ionic strength, composition, and pH of seawater, compared with freshwater, have potential effects on the partitioning of a chemical with other compartments. To a large extent, these effects are associated with differences in water solubility and/or speciation of the chemical, compared with freshwater. The relatively high levels of dissolved inorganic salts in seawater generally decrease the solubility of a chemical (referred to as ‘salting-out’), by about 10-50% for non-polar organic compounds but by a smaller fraction for more polar compounds (Schwarzenbach et al., 1993). A recent review found a typical reduction factor of 1.36 (Xie et al., 1997).

For non-ionisable organic substances, the decreased solubility in seawater, compared with freshwater, is expected to result in proportional increases in the partition coefficients between water and octanol, organic carbon and air. However, considering the uncertainty in measured partition values and the uncertainty associated with the frequent need to predict some or all of the partition coefficients, the differences attributable to the seawater environment (less than a factor of 2) are unlikely to be significant in risk assessment. Thus, unless measured seawater data

of equal reliability are available, freshwater data can be used for non-ionisable organic compounds without adjustment for the marine environment.

For ionisable organic compounds, as for freshwater, the pH of the environment will affect the water solubility and partitioning of the substance. There is some evidence that the degree of dissociation may also be directly affected by the ionic strength of seawater (Esser and Moser, 1982). However, the resulting shift in the dissociation curve is relatively small compared with that which can occur due to pH for substances with dissociation constants close to the marine water pH. It may, therefore, be preferable to obtain realistic measurements by use of seawater instead of deionised water. Another option is to measure the log Kow dependency of the pH directly (cf. the new draft OECD guideline 122 "Log Kow pH-metric method for ionisable substances" (OECD, 2000g). Because the pH of seawater (approximately 8) tends to be more constant than that of freshwater, the procedure to correct partition coefficients for ionisable substances, as described in Appendix XI**,** may however be considered sufficiently reliable for marine conditions.

For inorganic chemicals such as metals, the form or speciation of the substance can be directly affected by the ionic composition of seawater, which may have a considerable influence on both solubility and partitioning. On a case-by-case basis, there may be sufficient information available to allow the relevant partition coefficient in seawater to be calculated from the freshwater data; otherwise, measurements under marine conditions may be necessary.

4.2.3 Marine degradation

4.2.3.1 Abiotic degradation

Abiotic degradation (i.e. hydrolysis and photolysis) in marine environments should be assessed in a similar manner to abiotic degradation in freshwater environments except that the different physico-chemical conditions in marine environments should be taken into account. In particular the stable pH of about 8 and the generally lower temperature of in average 9°C (282 K) should be considered.

4.2.3.2 Biotic degradation

The rate of biodegradation in the various marine environments depends primarily on the presence of competent degraders, the concentration and the intrinsic properties of the chemical in question, the concentration of nutrients and organic matter and the presence of molecular oxygen. These factors vary significantly between various marine environments.

In estuarine environments, the supply of xenobiotics, nutrients and organic matter is much higher than in more distant marine environments. These factors enhance the probability that biodegradation of xenobiotics occurs with a greater rate in estuaries than is the case in more distant marine environments. Furthermore, estuarine and coastal environments are often turbulent and characterised by a constant sedimentation and re-suspension of sediment particles including microorganisms and nutrients, which increase the biodegradation potential in these environments compared to marine environments with a greater water depth. The presence of suspended particles and surfaces for attachment may favour the degradation of xenobiotics in estuarine environments.

ECETOC (1993) reviewed existing biodegradation data for the marine environments. They showed that the biodegradation in estuaries was approximately a factor 4 lower than in freshwater environments for a variety of substances: Linear Alkylbenzene-Sulfonates, Linear Alkyl-Ethoxylates, m-cresol, chlorobenzenes, p-nitrophenol glutamate, hexadecane, and methylparathion. However, for substances known to be very rapidly biodegradable (such as sodium acetate, sodium benzoate and sodium dodecylsulphate), the rates were similar in estuarine and freshwater environments. In this section the average degradation potential in estuarine environments is assumed to be similar to the degradation potential in freshwater environments.

Further away from the land-based sources of xenobiotics and allochthonous material the conditions for microorganisms are less favourable than close to land. The adaptation pressure is low due to much lower concentrations of xenobiotics as a result of degradation and dilution. Moreover, the environment can in general be characterised as oligotrophic, and the concentrations of nutrients and organic matter are lower than in marine environments closer to land. Because of their low concentrations, the xenobiotics are hardly degraded as primary substrates, and due to the relatively low microbial activity the degradation of xenobiotics as secondary substrates is assumed to be limited. This implies that the degradation potential in distant marine environments is anticipated to be much lower than the degradation potential in estuaries.

A special case is areas with offshore-based sources as, e.g., oil platforms. It may be assumed that the microorganisms associated with the sediment may be more or less adapted to degradation of chemicals that are continuously emitted from these sources. However, several factors, like e.g. nutrient limitation, may limit the biodegradation potential compared to the situation close to land. Furthermore, microorganisms in the water column will to a large extent drift with the currents and, therefore, a development of stable communities of competent degraders is impeded.

Most marine sediments are anaerobic below the upper 0-5 mm. The assessment of the biodegradation in marine sediments should ideally be based on results from investigations simulating these conditions. If not available, other approaches may be used, e.g.:

- an approach similar to the one used for freshwater sediments could be used, i.e. to use a scenario consisting of a 30 mm thick sediment layer of which the upper 3 mm are considered aerobic and the remaining part anaerobic. If separate degradation rates are available for aerobic and anaerobic sediment, these could be used for estimating the half-life. If only data on aerobic degradation in sediment (or soil) is available, no degradation in the anaerobic compartment should be assumed and consequently, a 10 times longer half-life than the half-life in aerobic sediment (or soil) should be used.
- anaerobic screening tests may be performed using a sediment inoculum (Horowitz et al., 1982; Madsen et al., 1995), and the observed biodegradability may then be used as an indication of the potential biodegradability of the substance in anaerobic sediment. Degradation rates should be derived by expert judgement.
- if no degradation data from studies with sediment or soil are available, the use of data on degradation in water could be considered. The degradation potential in the upper aerobic sediment layer is generally assumed to be similar to the degradation potential in the overlying water. However, the possible very low bioavailability in the sediment of highly hydrophobic and/or poorly water-soluble substances should be taken into consideration as is done also for freshwater sediments.

4.2.3.3 Marine biodegradation simulation tests

As a general rule, degradation rates or half-lives determined in tests simulating the conditions in the actual aquatic environment should be considered for use whenever available. Expert judgement of the validity and quality of the test data is necessary. The origin (e.g. relevance of sampling site) of the seawater/sediment inoculum shall always be evaluated in connection with assessment and use of simulation test results. Biotransformation (identification of metabolisation pathways and major metabolites) and mineralisation data may be derived from one of the standardised simulation tests by using samples from the particular environment as inoculum. Standardised simulation test methods for various marine compartments are:

- *Aquatic (pelagic) compartment*: ISO/DIS 14592-1 "Evaluation of the aerobic biodegradability of organic compounds at low concentrations – Part 1" (draft method 2001) The ISO method has been the basis for a proposal for a new OECD guideline "Simulation test - Aerobic transformation in surface water" (OECD, 2001d);
- *Turbid aquatic/sediment dispersed compartment*: ISO/DIS 14592-2 "Evaluation of the aerobic biodegradability of organic compounds at low concentrations – Part 2" (draft method, 2001b) and OECD 308: "Aerobic and anaerobic transformation in aquatic sediment systems" (aerobic test) (draft guideline, OECD, 2000c; draft Annex V C.24);
- *Anaerobic sediment compartment*: OECD 308 "Aerobic and anaerobic transformation in aquatic sediment systems" (strictly anaerobic test) (draft guideline, OECD, 2000c; draft Annex V C.24). Data from anaerobic screening tests conducted with digested sewage sludge (e.g. ISO 11734, 1994) cannot be used for predicting the degradation potential in sediments.

4.2.3.4 Use of biodegradation screening test data

For most chemicals, however, no test data from such simulation tests are yet available. For many chemicals only data from screening tests are available. This may be data from marine biodegradation screening tests or freshwater biodegradation screening tests. Marine screening tests may be:

- the OECD 306 "Biodegradability in Seawater" test (OECD, 1992e) comprises two methods, the Shake Flask Method and the Closed Bottle Method. These tests are seawater variants of the Modified OECD Screening Test (EU Annex V C.4-B and OECD 301E, 1992f) and Closed Bottle Test (EU Annex V C.4-E and OECD 301D, 1992f), respectively, the main difference being the use of a marine inoculum.
- three additional screening tests were subjected for a ring test initiated by the OSPAR Commission in 1995-96. The tests are the "Marine CO2 Evolution Test", the "Marine BODIS Test" and the "Marine CO2 Headspace Test". The results of the ring test were reported by Elf & IARE (1996).

When only results from marine or freshwater biodegradation screening tests are available, it is recommended to use the default mineralisation half-lives for the pelagic compartment as specified in **Table 24**.

Table 24 Recommended mineralisation half-lives (days) for use in marine risk assessment when only screening test data are available

	Freshwater [1)]	**Estuaries** [4)]	**Other marine environments** [5)]
Degradable in marine screening test	N.a.	15	50

Readily degradable [2)]	15	15	50
Readily degradable, but failing 10-d window	50	50	150
Inherently degradable [3)]	150	150	∞
Persistent	∞	∞	∞

Notes to Table 24:

1) Half-lives from Table 7.
2) Pass level >70% DOC removal or > 60% ThOD in 28 days. Not applicable for freshwater.
3) A half-life of 150 days may be used only for those inherently degradable substances that are quickly mineralised in the MITI II or the Zahn Wellens Test (cf. TGD Chapter 2.3.6). The half-life of 150 days is not fully scientifically justifiable (cf. TGD Chapter 2.3.6), but reflects a "guesstimate consensus" between a number of experts.
4) Also including shallow marine water closest to the coastline
5) The half-lives mentioned under this heading are normally to be used in the regional assessment (coastal model) as described in Section 4.2.5.

The half-lives for the marine environments that are described in **Table 24** are provisional recommendations, which should be reconsidered, when sufficient data for degradation of different substances in screening tests and simulation tests have been evaluated. The basis for the recommendation is the assumption that the degradation of xenobiotics in freshwater and estuarine waters in general can be described by similar degradation rates, whereas the degradation rates are lower in other marine environments more distant from the coastline (Here the half-life is suggested to be increased by a factor of three relative to estuaries for readily biodegradable substances and even more for more slowly degradable substances, see **Table 24**).

4.2.4 Local Assessment

4.2.4.1 Introduction

Usually releases to the environment stem from a point source leading to a locally high environmental concentration of the substance. The highest risk resulting from discharges, emissions and losses of a chemical into the environment is expected to be at this local scale close to the point of emission. It should be recognised that this might not always be the case and that other local high concentrations can arise some distance from the point of an emission due to marine currents, transport and deposition of sediments etc. Where this is considered possible for a local emission, specific modelling or measurements may be necessary. Since the aquatic concentrations are highest at the point of emission, risks may be adequately assessed, at this local scale, using the existing methodologies.

In addition to the inland sources of emission, there may also be direct discharges to the marine environment. Thus, releases can occur from point sources:

- to estuaries, either by direct discharges or from inland sources via riverine inputs (or both);
- to coastal areas;
- to harbour areas from port activity and shipping;
- to open sea e.g. from offshore oil and gas installations and from ships;
- atmospheric deposition.

4.2.4.2 Calculation of PEClocal for the aquatic compartment

In the current procedure of inland environmental risk assessment, the use of marine exposure scenarios had become necessary whenever site-specific assessments were performed for a large number of industrial sites, of which some actually discharge directly to the sea. A risk assessment for the marine environment on a local scale was therefore only performed for specific sites identified as releasing directly into the sea. In the context of a dedicated methodology for marine risk assessment, a more generic exposure assessment for any given use is necessary.

While in some countries with long coastlines, the number of industrial sites discharging wastewater to the sea is low compared with the overall number of sites (e.g. 5 – 10% in France; IFEN, 1997), it can be very high in others (e.g. 58 % in Sweden; SCB, 2000). It is therefore assumed that for all uses of a given chemical substance, potential local releases to the marine environment can occur and, hence, it is necessary to perform a generic local exposure assessment for the local marine environment.

As for inland risk assessment, the calculation of the PEClocal depends mainly on two parameters: dilution and the presence (or absence) of a STP. Both of these parameters have large influences on the local concentration ($Clocal_{seawater}$).

Regarding the presence or absence of a STP, conflicting information is available. Experience with the risk assessment of existing substances has shown that for chemical processing sites located on the coast, the probability that the effluents are treated in a biological treatment plant is much lower than for sites situated in land (see e.g., risk assessment reports for acrylonitrile, cyclohexane or methylene dianiline). This is confirmed by a survey performed by HELCOM (1998). While most industrial effluents from sites located on the Baltic Sea coast were treated (up to 98 %), the report did not contain detailed information on the treatment used from all contracting parties of HELCOM. However, from the data compiled in Sweden it appears that less than 50% of the industrial wastewater discharged passes a biological treatment step. On the other hand, statistics regarding treatment of municipal wastewater show that the treatment rate of municipal wastewater from coastal municipalities is not different from overall treatment rates (e.g. IFEN, 1997; HELCOM, 1998). On the other hand, four EU Member States have applied Article 6 of Directive 91/271 allowing them to declare marine areas non sensitive to urban wastewater meaning that they don't have to treat the wastewater biologically but only mechanically.

It is therefore proposed, for a default assessment, that in a local setting, industrial effluents (which may have been subject to some treatment on-site) are not treated in a municipal biological STP. It is recognised though that the situation regarding the treatment of industrial effluents is evolving rapidly and the present scenario could be revised in the near future. When there is specific information available for a certain site that specific treatment facilities are available this information needs to be assessed and can be used to override the default

assumption. In practice this information is often available for production and/or large processing sites. It may also be possible to assume the presence of connection to an STP for certain industry and/or use categories if appropriate justification about the general connection frequency to the STP for that specific industry is provided. For releases to municipal wastewater of substances that are used for private or public use (substances belonging to IC5 and IC6, Appendix I), however, it can be assumed that the degree of treatment in a biological STP corresponds to the inland scenario (see Section 2.3.7.1).

For discharges to a coastal zone, local dilution will be greater than in a freshwater river. First, initial dilution may occur if the density between the effluent and the saline receiving medium differs (Lewis, 1997). The initial dilution factor is usually around 10. Further dilution due to currents can also be assumed, particularly if the point of release is subject to tidal influences. In the Baltic or the Mediterranean sea, where there are almost no tidal influences compared to the Atlantic Ocean or the North Sea, only initial dilution may occur on calm days, but normally, further dilution due to currents is probable. Dilution factors of more than 500 have been determined from model simulations (based on current measurements) in the North Sea, 200 m away from the discharge point (e.g. Pedersen et al., 1994).

A dilution factor for discharges to a coastal zone of 100 may then tentatively be assumed, which seems to be representative of a realistic worst case. The same estimation method as for inland exposure assessment can then be used to obtain the local concentration in seawater ($Clocal_{seawater}$, see Section 2.3.8.3, equations 45-49).

In certain circumstances, it may be possible to identify specific emission points which would allow the use of more precise information regarding the available distribution and fate processes. Such “site-specific” assessments should only be used when it is known that all the emissions emanating from the particular point in the life-cycle, e.g. manufacture, arise from a limited number of specific and identifiable points. In these circumstances each specific point of release will need to be assessed individually. If it is not possible to make this judgement, then the default assumptions should be applied. In “site-specific” assessments, due account can be taken of the true dilution available to the given emission as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC. Normally, only dilution and adsorption to suspended sediment need be considered but site-specific conditions may indicate that valid local distribution models can be used.

For estuaries, which are influenced by currents and tidal movements, it is assumed as a first approach that they are covered by either the inland or the marine risk assessment. Thus, no specific assessment is proposed.

Then, the local concentration in seawater can be obtained with:

$$Clocal_{seawater} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION} \quad (83)$$

Explanation of symbols

$Clocal_{eff}$	concentration of the substance in the STP effluent	[mg · l^{-1}]	eq. (33)
Kp_{susp}	solids-water partitioning coefficient of suspended matter	[l · kg^{-1}]	eq. (24)
$SUSP_{water}$	concentration of suspended matter in the seawater	[mg · l^{-1}]	15
DILUTION	dilution factor	[-]	100
$Clocal_{seawater}$	local concentration in seawater during emission episode	[mg · l^{-1}]	

Kp_{susp} is derived as for inland risk assessment. For a specific estimation of the partitioning behaviour of substances in saltwater environments see Section 4.2.2.

It is recognised that the dilution available to a discharge will also be related to the actual volume of that discharge. In the freshwater scenario, this discharge volume is standardised to a volume of 2,000 m^3/day ie. the outflow from a standard STP. It is therefore proposed that the discharge volume to the marine environment is also normalised at 2,000 m^3/day such that the quantity of the substance discharged (in kg/day) is assumed, for modelling purposes, to be diluted into this volume prior to discharge.

For indirect human exposure and secondary poisoning, an annual average concentration in surface water is calculated:

$$Clocal_{seawater,ann} = Clocal_{seawater} \cdot \frac{Temission}{365} \tag{84}$$

Explanation of symbols

$Clocal_{seawater}$	local concentration in seawater during emission episode	[mg · l^{-1}]	eq. (83)
Temission	number of days per year that the emission takes place	[d · yr^{-1}]	App. IB
$Clocal_{seawater,ann}$	annual average local concentration in seawater	[mg · l^{-1}]	

The concentration at the regional scale ($PECregional_{seawater}$) is used as background concentration for the local scale. Therefore, these concentrations are summed:

$$PEClocal_{seawater} = Clocal_{seawater} + PECregional_{seawater} \tag{85}$$

$$PEClocal_{seawater,ann} = Clocal_{seawater,ann} + PECregional_{seawater} \tag{86}$$

Explanation of symbols

$Clocal_{seawater}$	local concentration in seawater during episode	[mg · l^{-1}]	eq. (83)
$Clocal_{seawater,ann}$	annual average concentration in seawater	[mg · l^{-1}]	eq. (84)
$PECregional_{seawater}$	regional concentration in seawater	[mg · l^{-1}]	4.2.5
$PEClocal_{seawater}$	predicted environmental concentration during episode	[mg · l^{-1}]	
$PEClocal_{seawater,ann}$	annual average predicted environmental concentration	[mg · l^{-1}]	

If relevant site-specific information is available, it can be used to improve the assessment. Some significantly different exposure situations need to be reviewed though:

- substances released from offshore platforms. A harmonised mandatory control system for the use and reduction of the discharge of offshore chemicals is already agreed within OSPAR (OSPAR, 2000a;2000b). For this specific exposure situation within the EU legislation, the methodology proposed by OSPAR can be taken into consideration[5];
- substances released from harbours, marinas, fish farms and dry-docks. Specific scenarios will have to be developed for these situations, which are most relevant for biocides.

4.2.4.3 Calculation of PEClocal for the sediment compartment.

The concentration in freshly deposited sediment is taken as the PEC for sediment; therefore the properties of suspended matter are used. The concentration in bulk sediment can be derived from the corresponding water body concentration, assuming a thermo-dynamic partitioning equilibrium (Di Toro et al., 1991):

$$PEClocal_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PEClocal_{seawater} \cdot 1000 \qquad (87)$$

Explanation of symbols

$PEClocal_{seawater}$	concentration in seawater during emission episode	$[mg \cdot l^{-1}]$	
$K_{susp\text{-}water}$	suspended matter-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	eq. (24)
RHO_{susp}	bulk density of suspended matter	$[kg \cdot m^{-3}]$	eq. (18)
$PEClocal_{sed}$	predicted environmental concentration in sediment	$[mg \cdot kg^{-1}]$	

Highly adsorptive substances may not be considered adequately with the approach described above, as they are often not in equilibrium distribution between water and suspended matter because of their cohesion to suspended matter; however they may be desorbed after ingestion by benthic organisms.

Suspended matter exposed to local releases can subsequently be transported over long distances and deposited to sediment in distant areas. Therefore, it is possible that areas unrelated to local settings are exposed to the same sediment concentrations as would be expected only in the immediate vicinity of the releases. This has especially to be taken into account when comparing measured concentrations to estimated concentrations.

4.2.5 Regional assessment

For the release estimation of substances, a distinction is usually made between substances that are emitted through point sources to which specific locations can be assigned, and substances that enter the environment through diffuse releases.

Point source releases may have a major impact on the environmental concentration on a local scale (PEClocal) and contribute to the environmental concentrations on a larger scale (PECregional). Like with the freshwater environment for the marine situation it is necessary to

[5] The methodology for assessing releases from platforms (e.g. CHARM-model) that has been developed in the context of these OSPAR decisions was not re-discussed in the context of the development of the present guidance document for marine risk assessment.

evaluate the impact of substances that are released from point and diffuse sources over a wider area. The PECregional is supposed to take into account the further distribution and fate of a chemical upon release. The resulting PECregional is assumed to be a steady-state concentration of the substance.

The regional system for the freshwater environment is a relatively large area of 200 by 200 km which consists of 97% of soil and 3% of water. This system is surrounded by a larger area of the size of Europe, called the continent (see Sections 2.1.2 and 2.3.8.7). If for the marine region an area of similar size would be chosen where the water of the freshwater region would enter into, the resulting concentrations would be around 0.1% of the freshwater concentrations, mainly due to the dilution of the freshwater in the much larger seawater region.

To assess the potential impacts of multiple point and diffuse sources of substances on the marine environment a river plume in coastal sea water is considered as a marine regional generic environment as follows:

An area of coastal sea that receives all the water from the rivers from the regional system. This seawater compartment is exchanging chemical with the continental seawater compartment by dispersion and advection (a current of seawater flowing in a certain direction). The size of the coastal compartment is 40 km long, 10 km wide and 10 m deep. In addition to the input from the regional river water it receives 1% of the direct emissions from the inland sources which is supposed to represent a relevant fraction of the sources that are located near the sea and also have direct emissions into the sea compartment. Most of the relevant characteristics of the coastal compartment are similar to the freshwater compartment apart from the suspended matter concentration that is set to 5 mg/l. In the absence of specific information (e.g. from marine simulation tests) it is assumed that the biodegradation rate in the water column is approximately three times lower than in freshwater as described in Section 7.3. This scenario is shown in **Figure 15**.

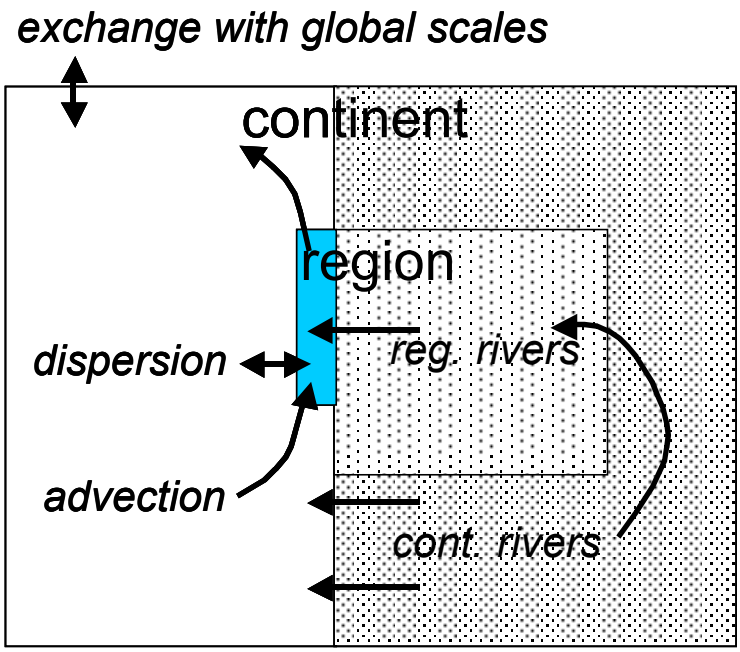

Figure 15 Coastal sea scenario.

This scenario can be modelled with the multi-media fate model that is used for the freshwater PEC calculations, modified to allow dispersive exchange between the coastal zone to the continental sea water. By default, mixing of river water into the coastal sea gives a dilution factor of approximately 10. As a result concentrations in coastal seawater are expected to be a factor of 10 (for conservative chemicals) or more (for chemicals that react, volatilize or sediment) lower than in river water. The extent of degradation, volatilization, etc. in this coastal sea scenario is adequately modeled using the multi-media model.

More details on the features of these models can be found in the section on calculation of PECregional for the freshwater environment (Section 2.3.8.7.)[6].

The calculation of PECregional according to this scenario provides the results for the generic risk assessment that is necessary for the risk evaluation for new and existing substances and biocides. Sufficient information on sources and emissions and site-specific information on the suspended matter concentration, the flow rate and the dispersion velocity may be available so the generic assessment can be made more site-specific by overriding some of the default parameters or even can be replaced by site-specific models. The dispersion velocity greatly affects all calculated concentrations, while in addition the suspended matter content further affects the dissolved concentration in seawater for chemicals with high log Kow. For the marine environment, models are available that can be used to assess the concentrations in certain specific compartments (bays, estuaries, regions) of the marine environment to which specific industrial sites discharge wastewater.

4.3 MARINE EFFECTS ASSESSMENT

4.3.1 Effects Assessment for the aquatic compartment

4.3.1.1 Introduction

Historically, the patterns of chemical production and usage resulting from urban and industrial development have led to the freshwater environment being considered to be the hydrosphere most at risk from these substances. Consequently, most regulatory schemes for evaluating the hazards and risks posed by new and existing substances have focussed primarily on the protection of freshwater communities. As a result there is a considerable body of data on the ecotoxicity of chemical substances to freshwater organisms (ECETOC, 1994a)[7].

Where there is a need to assess the potential impact of substances entering estuarine and marine waters, any hazard or risk assessment should ideally be based upon data generated using a range of ecologically relevant saltwater species (for example algae, invertebrates and fish). This is particularly important given the greater diversity of species (particularly invertebrates) present in

[6] A default length:width ratio of the coastal marine compartment has been set at 4:1. Assuming that this reflects the plume shape in the generic assessment situation, this implies a ratio between the advective sea current along the coast and the dispersive transport velocity perpendicular to that. If, in addition to the compartment dimensions, a value is chosen for the sea current, the value of the lateral dispersion coefficient follows, or *vice versa*. If then a value for the freshwater discharge into the coastal marine compartment is set too, mixing of freshwater with coastal seawater is determined completely. In the generic regional model the river discharges approximately 1000 m^3/s into the continental model. With the dimensions of the sea compartment set to 40,000 m · 10,000 m · 10 m, and a suggested default value for the sea current of 0.03 m/s, taking into account the necessary dispersion coefficient of 50 m^2/s, the freshwater content of the sea water inside the selected box would become approximately 10%.
It should be noted that river water plumes in coastal waters vary greatly with local conditions (river flow, sea current, tide, depth, etc.). Prediction of site-specific dilution of river water into coastal seawater requires site-specific knowledge of flows and salinity distributions. Rhine and Meuse water (2,000 m^3/s) are known to mix with a sea current of 0.035 m/s in the southern North Sea, yielding a very long-streched plume with approximately 20% river water in the first 10 km of the coast. A dispersion coefficient of 20 m^2/s adequately describes this situation. The Amazon river is known for its great plume.

[7] The ECETOC database consists of 2,203 entries on 361 chemicals, covering 121 species. Data on freshwater species accounted for 1862 entries (84.5%) while data for saltwater (estuarine/marine) species accounted for 341 entries (15.5%).

marine waters, relative to freshwaters (cf. Appendix XIV). There are also circumstances, however, where the special conditions existing in a particular environment such as that existing in the Baltic Sea, give rise to a reduced or limited species diversity and/or specific stresses such as low or variable salinity. In such circumstances of low species diversity, adverse impacts in individual species can have devastating impacts on the specialised ecosystem. Thus, while high species diversity may lead to a wide sensitivity distribution, but also considerable functional overlap, low species diversity may result in a lower sensitivity distribution but increase the ecosystem function dependency on individual keystone species.

In both cases, the effects assessment must use, where possible, data relevant to the environmental compartment that is considered. However, compared to the situation for freshwaters, there are relatively few data on the effects of chemical substances on estuarine and marine organisms. Therefore, in practice there will be situations where saltwater toxicity data are needed for hazard/risk assessments, but may not be available. In these situations it may be necessary to use freshwater data *in lieu* of data for estuarine/marine species (Schobben et al*.,* 1994; Karman et al*.,* 1998). In using data on freshwater species to characterise the risk in the marine waters, a clear understanding of the comparability of effects data generated on both types of species is necessary. Furthermore, there is some evidence, e.g. for some metals, that species living in brackish water are more susceptible because of the salinity (osmotic) stress they have to endure in contrast to those of the same species living in truly marine conditions. Under these circumstances the applicability of the toxicity data needs to be considered on a case-by-case basis.

4.3.1.2 Evaluation of data

It has been recognised for many years that there is a wider diversity of taxonomic groups (particularly invertebrates) in saltwaters compared to freshwaters and that many groups are only found in marine waters (see Russell and Yonge, 1928; Tait, 1978). Moss (1988) stated that 56 phyla were present in marine waters compared to 41 in freshwaters. No phyla are confined to freshwaters only while 15 phyla are found only in marine waters. These differences are partly due to the fact that multicellular animals originated in the seas and they have been well populated since the earliest fossil records.

Nevertheless, an important part of any evaluation of data must involve an assessment of the usefulness of the main body of freshwater ecotoxicity data in predicting effects in the marine environment. Where such data can be used, the focus of further investigation can concentrate on additional factors which specifically characterise the marine conditions. Studies conducted on the comparability of sensitivity of freshwater and marine species have been hampered by the low level of substances for which a comparable dataset has been available. Nevertheless where such data are available, it has tended to show that there is no systematic bias in sensitivity where comparable tests and endpoints are paired. A recent report which collated much of the available data confirmed these findings (ECETOC, 2000). Based on the currently available data, it can be concluded that:

- overall, the data reviewed and current marine risk assessment practice suggest a reasonable correlation between the ecotoxicological responses of freshwater and saltwater biota - at least for the usual aquatic taxa (i.e., fish, crustacea, algae). No marked difference in sensitivity between freshwater and saltwater biota appears that systematically applies across all three trophic levels considered;

- where evaluated, differences between trophic levels within each medium were generally as significant or even more marked than between media. Such variation is implicitly assumed in the use of assessment factors in current risk assessment practice;
- where differences in the apparent sensitivity of freshwater and marine biota were observed for individual compounds, such differences were consistently within a factor of 10 (<1 log unit) and usually somewhat less;
- average differences in sensitivity for such paired species comparisons were typically within a factor of ~2;
- however, within trophic levels differences larger than a factor of 10 were shown for several metals and pesticides indicating that for these substances fresh water and saltwater data should not be pooled for effects assessment and PNEC derivation.

The use of freshwater acute effects data *in lieu* of or in addition to saltwater effects data for risk assessment purposes is not contra-indicated by the empirical data reviewed. Use of pooled data is therefore recommended. Under such circumstances, PNEC values should be derived from the most sensitive endpoint regardless of the medium.

No comparison of long-term effects data has been made due to the lack of suitable data but again there are no reasons to believe that a systematic bias to freshwater or marine species would exist. Therefore it is proposed that data on freshwater or marine fish, crustacea and algae be used interchangeably for evaluation of the risks to either compartment.

4.3.1.3 Derivation of PNEC

The greater species diversity in the marine environment, compared to freshwaters (see Appendix XIV), including the presence of a number of taxa that occur only in that environment, may mean that the distribution of sensitivities of species is broader. It is necessary to consider, therefore, whether the three-taxa model offers sufficient certainty that sensitive species will be covered using the assessment factors developed for the freshwater systems. Since it is not possible to make a clear judgement on the basis of available data, it is considered prudent to assume that this greater diversity of taxa will produce a broader distribution of species sensitivity. Thus, where only data for freshwater or saltwater algae, crustaceans and fish is available a higher assessment factor than that for the derivation of $PNEC_{water}$ for freshwaters should be applied, to reflect the greater uncertainty in the extrapolation. Where data is available for additional taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a dataset can be lowered. Test protocols for these groups are available from organisations such as the American Society for Testing and Materials, the International Council for the Exploration of the Seas and the United States Environmental Protection Agency (OECD, 1998a). The assessment factors given are based on current scientific understanding on the species comparability of toxicity between freshwater and saltwater species and the issue of differences in diversity in freshwaters and saltwaters. These may need to be revisited as additional information becomes available.

It is recognised that the assumption of a greater species sensitivity distribution covering the additional marine taxa is based on limited data and is precautionary. The generation of additional toxicity data on marine species may allow this assumption to be further refined such that lower or higher assessment factors may be considered following a systematic review of accumulating evidence.

The additional assessment factor is also considered sufficient to cover the situations noted above where low species diversity may result in high ecosystem dependency on individual species.

The assessment factors decrease in magnitude from higher values for short-term acute studies from which L(E)C50 values have been derived to lower values for long-term chronic studies from which NOECs have been derived. For long-term studies the magnitude of the assessment factors also decreases as information on a wider range of species becomes available. The assessment factors described in **Table 25** are those that would normally be applied to the datasets available. There are some circumstances, however, where expert judgement may be applied to the interpretation of a dataset which may allow a pragmatic approach to the application of the factors and the generation of new data. In each case where expert judgement is so applied, a full justification must be provided.

Table 25 Assessment factors proposed for deriving $PNEC_{water}$ for saltwater for different data sets

Data set	Assessment factor
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10,000 a)
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels, + two additional marine taxonomic groups (e.g. echinoderms, molluscs)	1000 b)
One long-term NOEC (from freshwater or saltwater crustacean reproduction or fish growth studies)	1000 b)
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish)	500 c)
Lowest long-term NOECs from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels	100 d)
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish) + one long-term NOEC from an additional marine taxonomic group (e.g. echinoderms, molluscs)	50
Lowest long-term NOECs from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels + two long-term NOECs from additional marine taxonomic groups (e.g. echinoderms, molluscs)	10

Notes to Table 25:

Evidence for varying the assessment factor should in general include a consideration of the availability of data from a wider selection of species covering additional feeding strategies/ life forms/ taxonomic groups other than those represented by the algal, crustacean and fish species (such as echinoderms or molluscs). This is especially the case, where data are available for additional taxonomic groups representative of marine species. More specific recommendations as with regard to issues to consider in relation to the data available and the size and variation of the assessment factor are indicated below.

When substantiated evidence exists that the substances may be disrupting the endocrine system of mammals, birds, aquatic or other wildlife species, it should be considered whether the assessment factor would also be sufficient to protect against effects caused by such a mode of action, or whether an increase of the factor would be appropriate.

a)

The use of a factor of 10,000 on short-term toxicity data is a conservative and protective factor and is designed to ensure that substances with the potential to cause adverse effects are identified in the effects assessment. It assumes that each of the identified uncertainties described above makes a significant contribution to the overall uncertainty.

For any given substance there may be evidence that this is not so, or that one particular component of the uncertainty is more important than any other. In these circumstances it may be necessary to vary this factor. This variation may lead to a raised or lowered assessment factor depending on the evidence available. Except for substances with intermittent release, as defined in Section 2.3.3.4, under no circumstances should a factor lower than 1000 be used in deriving a $PNEC_{water}$ for saltwater from short-term toxicity data.

Evidence for varying the assessment factor could include one or more of the following:

– evidence from structurally similar compounds which may demonstrate that a higher or lower factor may be appropriate.

- knowledge of the mode of action as some substances by virtue of their structure may be known to act in a non-specific manner. A lower factor may therefore be considered. Equally a known specific mode of action may lead to a higher factor.
- the availability of data from a variety of species covering the taxonomic groups of the base set species across at least three trophic levels. In such a case the assessment factors may only be lowered if multiple data points are available for the most sensitive taxonomic group (i.e. the group showing acute toxicity more than 10 times lower than for the other groups).

There are cases where a complete short-term dataset even for freshwater algal, crustacean and fish species will not be available, for example for substances which are produced at < 1 t/a (notifications according to Annex VII B of Directive 92/32). In these situations, the only data may be short-term L(E)C50 data for *Daphnia*. In these exceptional cases, the PNEC should be calculated with a factor of 10,000.

Variation from an assessment factor of 10000 should be fully reported with accompanying evidence.

b)

An assessment factor of 1000 applies where data from a wider selection of species are available covering additional taxonomic groups (such as echinoderms or molluscs) other than those represented by algal, crustacean and fish species; if at least data are available for two additional taxonomic groups representative of marine species.

An assessment factor of 1000 applies to a single long-term NOEC (freshwater or saltwater crustacean or fish) if this NOEC was generated for the taxonomic group showing the lowest L(E)C50 in the short-term algal, crustacean or fish tests.

If the only available long-term NOEC is from a species which does not have the lowest L(E)C50 in the short-term tests, it cannot be regarded as protective of other more sensitive species using the assessment factors available. Thus, the effects assessment is based on the short-term data with an assessment factor of 10,000. However, normally the lowest PNEC should prevail.

An assessment factor of 1000 applies also to the lowest of the two long-term NOECs covering two trophic levels (freshwater or saltwater algae and/or crustacean and/or fish) when such NOECs have not been generated for the species showing the lowest L(E)C50 of the short-term tests.

This should not apply in cases where the acutely most sensitive species has an L(E)C50-value lower than the lowest NOEC value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest L(E)C50 of the short-term tests.

c)

An assessment factor of 500 applies to the lowest of two NOECs covering two trophic levels (freshwater or saltwater algae and/or crustacean and/or fish) when such NOECs have been generated covering those trophic levels showing the lowest L(E)C50 in the short-term tests with these species. Consideration can be given to lowering this factor in the following circumstances:

- It may sometimes be possible to determine with a high probability that the most sensitive species covering fish, crustacea and algae has been examined, that is that a further longer-term NOEC from a third taxonomic group would not be lower than the data already available. In such circumstances an assessment factor of 100 would be justified;
- a reduced assessment factor (to 100 if only one short-term test, to 50 if two short-term tests on marine species are available) applied to the lowest NOEC from only two species may be appropriate where:
  - short-term tests for additional species representing marine taxonomic groups (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and;
  - it has been determined with a high probability that long-term NOECs generated for these marine groups would not be lower than that already obtained. This is particularly important if the substance does not have the potential to bioaccumulate.

An assessment factor of 500 also applies to the lowest of three NOECs covering three trophic levels, when such NOECs have not been generated from the taxonomic group showing the lowest L(E)C50 in short-term tests. This should, however, not apply in the case where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest L(E)C50 in the short-term tests.

d)

An assessment factor of 100 will be applied when longer-term toxicity NOECs are available from three freshwater or saltwater species (algae, crustaceans and fish) across three trophic levels.

The assessment factor may be reduced to a minimum of 10 in the following situations:

- where short-term tests for additional species representing marine taxonomic groups (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and it has been determined with a high probability that long-term NOECs generated for these species would not be lower than that already obtained;
- where short-term tests for additional taxonomic groups (for example echinoderms or molluscs) have indicated that one of these is the most sensitive group acutely and a long-term test has been carried out for that species. This will only apply when it has been determined with a high probability that additional NOECs generated from other taxa will not be lower than the NOECs already available.

A factor of 10 cannot be decreased on the basis of laboratory studies only.

Statistical extrapolation methods for calculation of PNEC for marine organisms could be used when sufficient data are available. More information on these methods and the prerequisites to apply them for risk assessment purposes can be found in Section 3.3.1.2.

4.3.2 Effects assessment for the sediment compartment

4.3.2.1 Introduction

Substances that are highly hydrophobic may be assessed as of low risk for pelagic fauna but can accumulate in sediments to concentrations at which they might exert significant toxic effects (SETAC, 1993). This may be of concern particular in the marine environment, where the sediment may act as a permanent sink for highly hydrophobic substances that can be accumulated to a large extent. Because marine sediment constitutes an important compartment of marine ecosystems it may be important to perform an effects assessment for the marine sediment compartment for those substances.

In principle the same strategy as applied to freshwater sediment is recommended (see Section 3.5) for the effects assessment of marine sediment). Several test methods on sediment are developed and used in Member States of the European Union. Most of the tests are used for sediment management purposes; only a few tests are conducted for risk assessment of substances. An inventory of tests with marine organisms for the evaluation of dredged material and sediments has been compiled by the Federal Environment Agency of Germany, UBA (Herbst and Nendza, 2000). It comprises of biotests with various species of marine organisms of different trophic levels on whole sediment, pore water or sediment extracts. In addition OECD has prepared a detailed review paper on aquatic ecotoxicity tests including marine sediment test methods (OECD, 1998a). Only whole sediment tests with infaunal and epibentic organisms are considered suitable for being used in a risk assessment of the marine sediment compartment. From examination of the UBA and OECD inventories it is clear that no fully internationally accepted, standardised test methods for whole sediment are currently available.

Most of the existing whole sediment tests measure acute toxicity; only a few measure long-term, sub-lethal endpoints. Only the latter tests are considered applicable to marine risk assessment because of the long-term exposure of benthic organisms to sediment-bound substances that occur under field conditions.

In Section 4.3.1 freshwater toxicity data are compared to marine and estuarine data. It is concluded that the use of freshwater acute effects data *in lieu* or together with saltwater effects data is acceptable for risk assessment purposes. Although it is not sure that this also applies to marine and freshwater sediment data, it is nevertheless recommended to use pooled marine and freshwater sediment toxicity data for effect assessment for the sediment compartment. However, when sufficient data for ecologically relevant saltwater species are available lower assessment factors can be applied.

4.3.2.2 Strategy for effects assessment for sediment organisms

Substances that are potentially capable of depositing on or sorbing to sediments to a significant extent have to be assessed for toxicity to sediment-dwelling organisms. In addition, marine sediment effects assessment is necessary for substances that are known to be persistent in marine

waters, and may accumulate in sediments over time. In general substances with a Koc < 500 – 1000 L/kg are not likely sorbed to sediment (SETAC, 1993). To avoid extensive testing of chemicals a log Koc or log Kow of ≥ 3 can be used as a trigger value for sediment effects assessment.

For most existing chemicals the number of toxicity data on infaunal and epibenthic organisms will be limited. As a screening approach the equilibrium method can be used to compensate for the lack of toxicity data if a $PEC_{marine\ sediment}$ can be determined on the basis of a measured concentration of the substance in water that is independent of the value of the Koc. If the PEC/PNEC determined using this method is > 1 then the need for testing with benthic organisms using spiked sediment should be considered.

It is not necessary to apply the equilibrium partitioning method to predicted environmental concentrations obtained from application of an exposure model when such a model will have used the same Koc or log Kow value as that used to predict the $PNEC_{sediment}$. The reason is that the resulting PEC/PNEC ratio for sediment will have the same value as for the water compartment. In this case no quantitative risk characterisation for marine sediment should be performed. Under these circumstances the assessment conducted for the aquatic compartment will also cover the sediment compartment for chemicals with a log Kow up to 5. For substances with a log Kow > 5 (or with a corresponding Koc), however, the PEC/PNEC ratio for the aquatic compartment is increased by a factor of 10. The increased factor is justified by the fact that the equilibrium partitioning method considers mainly the exposure via the water phase and does not include that potential additional accumulation via sediment ingestion may occur for certain types of sediment dwelling invertebrates (see Section 8.2.3).

Four situations can be distinguished for deriving a $PNEC_{sediment}$:

1. where only results from acute tests with benthic freshwater organisms are available (at least one) the risk assessment is performed both on basis of the tests and on the basis of the equilibrium partitioning method. The lowest $PNEC_{marine\ sediment}$ is then used for the risk characterisation.
2. where, in addition to the tests with freshwater benthic organisms, an acute toxicity test is performed with a marine benthic organism that is preferably representative of the same taxon that is judged to be the most sensitive in the freshwater tests. Under these circumstances an assessment factor of 1000 is applicable. A reduction of the assessment factor is only justified if sufficient long-term tests with sediment-dwelling organisms are available, and, if possible, where other evidence indicates that these tests include sensitive taxonomic groups. Also in this case a comparison with the screening approach has to be made and the lowest $PNEC_{sediment}$ should be used for the risk characterisation.
3. where long-term toxicity data are available for benthic freshwater organisms. Under this circumstance the $PNEC_{marine\ sediment}$ is calculated using assessment factors for long-term tests. This approach is explained in Section 4.3.2.4.
4. where long-term toxicity data are available for benthic freshwater *and* a minimum of two marine organisms. Under these circumstances a $PNEC_{marine\ sediment}$ is calculated using the lower assessment factors that are associated with data obtained from long-term tests. A $PNEC_{marine\ sediment}$ obtained from such data is preferred for risk assessment. This approach is explained in Section 4.3.2.4.

Table 18 in Section 3.5.2 presents an overview of different data configurations and explains how to use them for the risk characterisation for sediment. Attention should be paid to the fact that very often contaminants are not analysed in whole sediment but in a certain fraction of the

sediment, for example in the sediment fraction of particles < 63 μm. The organic carbon content of this fraction is typically 15-30% for marine sediment while for whole marine sediments it is generally less than 2%. It is important, for reasons of comparability of PEC and PNEC values, that the organic carbon content of sediment used for toxicity tests are comparable with those of actual marine sediments. If not there are likely to be concerns regarding the relative bioavailability of a substance in the different sediments.

4.3.2.3 Calculations of PNEC for marine sediment using the equilibrium method

In the absence of any ecotoxicological data for sediment-dwelling organisms, but with measured data to predict the $PEC_{marine\ sediment}$, the $PNEC_{marine\ sediment}$ may provisionally be calculated using the equilibrium partitioning method. This method uses the $PNEC_{saltwater}$ for aquatic organisms and the marine suspended matter/water partitioning coefficient. The assumptions that are made in this method are described in Section 3.5.3. Based on the equilibrium partitioning the following equation is applied:

$$PNEC_{marine-sediment} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PNEC_{saltwater} \cdot 1000 \qquad (88)$$

Explanation of symbols

$PNEC_{saltwater}$	Predicted No Effect Concentration in saltwater	$[mg \cdot l^{-1}]$	
RHO_{susp}	bulk density of suspended matter	$[kg \cdot m^{-3}]$	eq. (18)
$K_{susp\ water}$	partition coefficient suspended matter water	$[m^3 \cdot m^{-3}]$	eq. (24)
$PNEC_{marine\ sediment}$	Predicted No Effect Concentration in marine sediment	$[mg \cdot kg^{-1}]$	

In Section 3.5.2 a remark is made with respect to the calculation of $PNEC_{marine\ sediment}$ using the equilibrium partitioning method. The equilibrium partitioning method considers uptake via the water phase, while uptake may also occur via other exposure pathways such as ingestion of sediment or direct contact with sediment. This may be important, especially for chemicals that have a tendency to adsorb to sediment organic matter, for example those with a log Kow greater than 3. Direct uptake from marine sediment is also observed in studies with marine benthic organisms and may significantly contribute to the uptake of organic contaminants such as PAHs (Kaag, 1998). There is also however evidence from studies in soil and in marine sediment that the proportion of the total dose taken up through intake of sediment particles remains low for chemicals with a log Kow up to 5. From other studies it is obvious that feeding mode also influences uptake of substances (via water or ingestion of sediment). Furthermore the absorption of contaminants in the gastrointestinal tract has been found to be increased compared with absorption from the surrounding water (Mayer et al., 1996; Voparil and Mayer, 2000). However, no quantitative conclusions can be drawn from these studies regarding uptake of substances from sediment.

For substances with a log Kow greater than 5 (or with a corresponding Kp_{sed}) the equilibrium partitioning method is used in a modified way in order to take account of possible uptake via ingestion of sediment. Thus the resulting PEC/PNEC ratio is increased by a factor of 10 for these compounds. It should be borne in mind that this approach is considered as a screening level assessment of the risk to sediment dwelling organisms. If with this method a PEC/PNEC ratio > 1 is derived then tests, preferably long-term, with benthic organisms using spiked sediment have

to be conducted in order for a realistic risk assessment appropriate to the sediment compartment to be carried out.

4.3.2.4 Calculation of PNEC for marine sediment using assessment factors

If results from whole-sediment tests with benthic organisms are available the $PNEC_{marine\ sediment}$ has to be derived using assessment factors. In establishing the size of the assessment factors, a number of uncertainties have to be addressed (cf. Section 3.2). Due to the generally long-term exposure of benthic organisms to sediment-bound substances, long-term tests with sub-lethal endpoints like reproduction, growth, emergence, sediment avoidance and burrowing activity are regarded as most relevant.

In contrast to the concept applied to the pelagic marine compartment, it is only necessary to have results from one acute sediment test for the assessment factor of 10000 to apply. Furthermore if only results from short-term tests with freshwater sediment-dwelling organisms are available (at least one) an assessment factor of 10,000 is also applied to the lowest value. The $PNEC_{marine\ sediment}$ should also be calculated from the $PNEC_{saltwater}$ using the equilibrium-partitioning method.

If, in addition to the results of tests with freshwater benthic organisms, a result from an acute toxicity test with a marine benthic organism (preferably representative of the same taxa that is most sensitive in aquatic freshwater or saltwater tests) is available then an assessment factor of 1000 is applicable. Once again a $PNEC_{marine\ sediment}$ should also be calculated from the $PNEC_{saltwater}$ using the equilibrium partitioning method. A reduction of the assessment factor is only permitted if results from long-term tests with sediment-dwelling organisms are available.

A $PNEC_{marine\ sediment}$ is derived by application of the following assessment factors to the lowest LC50 value from acute tests:

Table 26 Assessment factors for derivation of $PNEC_{marine\ sediment}$ from short-term sediment toxicity tests

Available test results	Assessment factor	$PNEC_{marine\ sediment}$
One acute freshwater or marine test	10,000	Lowest of LC50 /10,000 and equilibrium-partitioning method
Two acute tests including a minimum of one marine test with an organism of a sensitive taxa	1000	Lowest of LC50 /1000 and equilibrium-partitioning method

A $PNEC_{marine\ sediment}$ is derived by application of the following assessment factors to the lowest NOEC/EC10 value from long-term tests:

Table 27 Assessment factors for derivation of $PNEC_{marine\ sediment}$ from long-term sediment toxicity tests

Available test results	Assessment factor [a)]
One long-term freshwater sediment test	1000
Two long-term freshwater sediment tests with species representing different living and feeding conditions	500
One long-term freshwater and one saltwater sediment test representing different living and feeding conditions	100
Three long-term sediment tests with species representing different living and feeding conditions	50
Three long-term tests with species representing different living and feeding conditions including a minimum of two tests with marine species	10

a) The general principles of notes (c) and (d) as applied to data on aquatic organisms (Section 4.3.1.3) shall also apply to sediment data. Additionally, where there is convincing evidence that the sensitivity of marine organisms is adequately covered by that available from freshwater species, the assessment factors used for freshwater sediment data may be applied. Such evidence may include data from long-term testing of freshwater and marine aquatic organisms, and must include data on specific marine taxa.

If no results from long-term tests with sediment organisms are available and the PEC/PNEC ratio derived from the results of short-term sediment tests or via the equilibrium partitioning method is a cause for concern then the need for long-term testing with sediment organisms should be considered.

Since there are no chronic marine sediment test methods that are internationally accepted the results from any tests should always be carefully evaluated. Several factors can contribute to variability in test results. Of major importance to sediment tests are the effects of grain size and organic carbon content of the sediment on the bioavailability of a substance. Sediment grain size can also be an important factor in tests for other reasons. For example, the extent to which bacteria can be adsorbed onto the sediment varies with particle size. Likewise, different species of amphipods prefer sediments with different particle size distributions. No satisfactory solution to the question which reference sediment should be considered appropriate is therefore currently available. One should thus consider the tolerance of a given species with regard to the grain size distribution of the sediments in question. Also spiking techniques have to be optimised because often water is spiked after spiking the sediment. In addition, more insight is needed in the uptake route of sediment bound contaminants in the organisms (exposure assessment).

Next to standardisation and test guidelines, it is necessary to further investigate the sensitivity, reproducibility and inter-laboratory variability of the tests. It must be mentioned that most available data on these facts concern the tests applied on field sediments, and not on spiked sediments.

Examples of sub-chronic and chronic toxicity tests with whole sediment are given in **Table 28**. Most of the tests have been developed for amphipods and polychaetes and some of them are recommended by the OECD (1998a). There is a need for chronic tests to be developed for Mollusca. Early life-stage tests with mussels and oysters are available for testing aqueous phases but no standardised test is available for testing whole marine sediment samples. Chronic tests that measure effects on community structure are also available but these tests seem to be very insensitive. Functional endpoints tests, e.g. nutrient release rates, have been used to assess the effects of contaminated sediments (Dahllöff et al., 1999).

A final point that should be borne in mind is that single-species toxicity tests do not take account of the interactions between the sediment inhabiting fauna and the fate or behaviour of chemical substances, caused by e.g. bioturbation (Ciarelli et al., 1999; 2000). No procedures are currently

available for assessing the significance of such interactions but it is clear that they could be of potential significance, particularly in respect of the bioavailability of a sediment contaminant.

Table 28 Acute and chronic whole sediment toxicity tests

Test organism	Acute or chronic test	Duration	Endpoints	Reference	
AMPHIPODS					
Corophium sp. (*C. volutator* or *C. arenarium*)	Chronic	28d	survival, growth and reproduction	ASTM (1993), Environment Canada (Burton, 1992), (OECD, 1998a recommended)	Degrader. Organisms can be field collected. Cultivation causes intermediate to high expenses Organism does not like coarse sediment. Low concern with regard to animal welfare Ecologically important organisms relevance for exposed ecosystems high. SOP [1)] available with field-collected organisms. Ringtested
Leptocheirus plumulosus	chronic	28 d	survival, growth and reproduction	ASTM (1993), Environment Canada (Burton, 1992), US EPA (1996)	Degrader grain size has a significant effect on survival, growth and reproduction. Survival is highest between 25% clay and 75% sand. Low concern with regard to animal welfare Ecologically important organisms relevance for exposed ecosystems very high SOP [1)] available with field-collected organisms. Ringtested
POLYCHAETES					
Nereis/Neanthes sp Neanthes arenaceodentatakan cultivated	subacute/ chronic	12 d - 28 d	survival - survival/growth	ASTM (1994)	Distributed widely throughout the world. Can be cultivated on the laboratory degrader Low concern with regard to animal welfare relevance for exposed ecosystems very high. SOP [1)] available, equipment and test species commercially available. Ringtested.

Table 28 continued overleaf

Table 28 continued Acute and chronic whole sediment toxicity tests

Test organism	Acute or chronic test	Duration	Endpoints	Reference	
POLYCHAETES (continued)					
Arenicola marina	chronic	28 d	Survival	ASTM (1994) (OECD, 1998a recommended)	Degrader, wide tolerance of sediment grain size. Organism is found extensively over the OSPAR and Helsinki conventions area; cultivation is difficult Low concern with regard to animal welfare relevance for exposed ecosystems very high. SOP 1) available, equipment and test species commercially available. Ringtested.
Arenicola marina	subacute	10	Casting rate	Thain and Bifield (2001)	see above row . Changes in feeding rate have consequences for sediment communities. SOP 1) available, equipment and test species commercially available. OSPAR ringtested
ECHINODERMES					
Echinocardium cordatum	acute/ subchronic	14 d	Survival	Stronkhorst, in press (OECD, 1998a recommended)	Degrader, SOP 1) available with field-collected organisms Ringtested
MICROCOSM					
Nematodes	chronic	60 d	community structure	(Austen and Somerfield, 1997)	

1) Standard operating procedure

4.3.3 Assessment of secondary poisoning

4.3.3.1 Introduction

The assessment of the potential impact of substances on top predators in the marine environment can be based, in principle, on the same methodology as that used for a freshwater scenario. As with freshwater ecosystems the accumulation of hydrophobic chemicals through the marine food chains may follow many different pathways along different trophic levels. This accumulation may result in toxic concentrations in predatory birds or mammals ingesting aquatic biota containing the chemical. This effect is called secondary poisoning and should in principle be assessed by comparing the measured or estimated concentrations in the tissues and organs of the top predators with the no-effect concentrations for these predators expressed as the internal dose. In practice, however, data on internal concentrations in wildlife animals are hardly ever available

and most no-effect levels are expressed in term of concentrations of the food that the organisms consume (i.e. in $mg \cdot kg^{-1}$ food). Therefore, the actual assessment is normally based on a comparison of the (predicted) concentration in the food of the top predator and the (predicted) no-effect concentration which is based on studies with laboratory animals. A distinction is made between the methodology used to assess the effects of substances whose effects can be related directly to bioconcentration (direct uptake via water) and those where also indirect uptake via the food may contribute significantly to the bioaccumulation.

Highly bioaccumulative substances have both a very high bioconcentration potential (log Kow typically >4.5 or BCF > 500) and are also resistant to biotransformation in animals. Biomagnification of such chemicals (increased food chain accumulation) is a major risk to the top predators of food webs, as the consumption of contaminated food is a major source of contaminants in predatory marine birds and mammals. In contrast the direct uptake of substances from the environment (that is from water and sediment) is only of minor relevance (Biddinger and Gloss, 1984; Opperhuizen, 1991). Factors that make these very hydrophobic substances of particular concern to the marine environment include longer food chains, migratory and reproductive aspects that may cause especially high exposure of progeny of marine species likely, long-life of many marine predators, and a higher fat content. However, whilst steady state levels in birds may be reached within weeks depending on the biological half-life of the chemical (Pearce et al., 1989), contamination levels in mammals may continually increase with age, with a plateau only being evident after several years (Thompson, 1990; Teigen et al., 1993).

No distinction can effectively be made between the spatial scales in the approach to the assessment since the predators will take food from sources spread across local and regional marine scenarios, as well as from the open sea. In the assessment it is therefore proposed to use a $PEC_{saltwater}$ based on the mean of the local and regional concentrations for the assessment of the local situation, and for the regional situation to apply a spatially broader scale. Given that marine predators may have a wider range of foraging and that the regional sea concentrations will normally be lower, this is considered as a reasonable worst-case assumption.

Bioaccumulation of metallic species is not considered explicitly in this section.

4.3.3.2 Assessment of bioaccumulation and secondary poisoning

The assessment scheme

The principal endpoints for the secondary poisoning assessment are the predators and top predators that prey on organisms that are in direct contact with the marine aqueous phase and receive the substances from this source. A relatively simple food chain is modelled which consists of the marine water phase, marine food, marine fish and two separate levels of predators. This food chain is visualised in **Figure 16**. As can be seen from this scheme risks for three different trophic levels need to be assessed:

1. *risks to marine fish:* No specific calculation needs to be performed for estimating the risk to marine fish as this is covered by the risk assessment for aquatic organisms.
2. *risks to marine predators:* The risk to marine predators is calculated as the ratio between the concentration in their food (marine fish) and the no-effect concentration for oral intake ($PNECoral_{predator}$). The concentration in the marine fish (C_{fish}) is obtained from bioconcentration of the substance from the aqueous phase and (for very hydrophobic substances) as a result of bioaccumulation from the food the fish consumes (which consists

of different types of aquatic organisms). Therefore, both a bioconcentration factor (BCF) and a biomagnification factor (BMF_1) are used to calculate C_{fish}. Note that for the BCF_{fish} also information for other organisms such as mussels may be considered.

3. *risks to marine top predators:* The risk to marine top-predators is calculated as the ratio between the concentration in their food (marine predators) and the no-effect concentration for oral intake ($PNECoral_{top\ predator}$). Since very hydrophobic substances may biomagnify in the tissue and organs of the predator, for the calculation of the internal concentration of the predator an additional biomagnification factor (BMF_2) must be applied. Note that no additional BMF factor for the top predator itself is required since the comparison between PECoral and PNECoral is not based on internal concentrations but on intake rates.

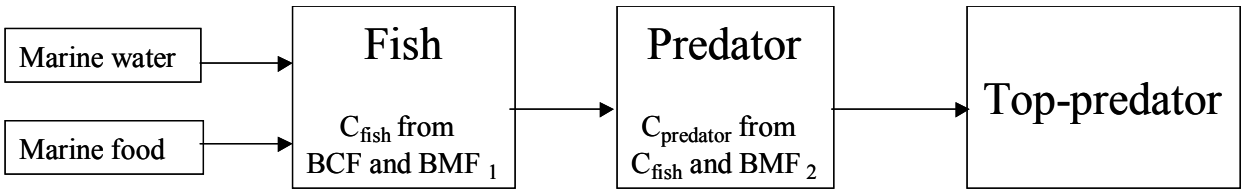

Figure 16: Secondary poisoning food chain

It is realised that food chains of the marine environment can be very long and complex and may consist of 5 or more trophic levels. The possible extent of bioaccumulation in marine food chains with more than the above three to four trophic levels should be evaluated case by case if necessary input data for such an evaluation is available, using the principles for the shorter food chain. Also if further data are available it may be possible to refine the assessment of secondary poisoning via marine food chains by employing more advanced modelling that takes the differences in for instance uptake and metabolic rates into account for the different trophic levels.

In the relatively simple food chain given above the concentration in the fish (i.e. the food for the fish-eater) ideally should take account of all possible exposure routes, but in most instances this will not be possible because it is not clear what contribution each potential exposure route makes to the overall body burden of a contaminant in fish species. Therefore for very hydrophobic substances a simple correction factor for potential biomagnification on top of the bioconcentration through the water phase is applied.

Calculation of PEC in food of predators

The actual calculation of the concentration of a chemical in the food of the predators and top predators will include the following steps:

$$PEC_{oral,predator} = PEC_{seawater} \cdot BCF_{fish} \cdot BMF_1 \tag{89}$$

$$PEC_{oral,toppredator} = PEC_{oral,predator} \cdot BMF_2 = PEC_{water} \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2 \tag{90}$$

Explanation of symbols

$PECoral_{predator}$	concentration in the food of the predator	$[mg \cdot kg^{-1}]$	
$PECoral_{top\ predator}$	concentration in the food of the top predator	$[mg \cdot kg^{-1}]$	
$PEC_{seawater}$	concentration in seawater	$[mg \cdot l^{-1}]$	
BCF_{fish}	bioconcentration factor	$[l \cdot kg^{-1}]$	eq. (73)
BMF_1	biomagnification factor in fish	[-]	Table 29
BMF_2	biomagnification factor in the predator	[-]	Table 29

The biomagnification factors used should, ideally, be based on measured values. However, the limited availability of such data means that in most instances the default values described below may have to be used. The use of a default value represents a screening approach designed to identify substances for which it may be necessary to obtain more detailed information on the biomagnification factor.

Although there may be relationships between the magnitude of the BMF and the log Kow of the substance under defined conditions, the available data are not conclusive. Other more complex intrinsic properties of substances than the lipophilicity (log Kow) seems to be important as well as the species under consideration (e.g. its biology in relation to uptake, metabolism etc.). As a simple screening approach, however, it seems reasonable to assume that for organic substances with a log Kow up to 4.5 biomagnification seems generally to be low and thus BMF = 1. For higher log Kow the biomagnification increases up to around log Kow 7 and then it decreases again to be low around log Kow 9 (Fisk et al., 1998). Based on data published by Rasmussen et al. (1990), Clark and Mackay (1991), Evans et al. (1991) and Fisk et al. (1998), the default BMF values in **Table 29** are suggested. If a BCF for fish is available, it is possible to use that as a trigger instead of log Kow. The BCF triggers recommended are less conservative than the log Kow triggers because they more realistically take the potential for metabolism in biota (i.e. fish) into account. Due to this increased relevance, the use of BCF as a trigger would take precedence over a trigger based on log Kow.

Table 29 Default BMF values for organic substances with different log Kow or BCF in fish

log Kow	BCF (fish)	BMF_1	BMF_2
<4.5	< 2,000	1	1
4.5 - < 5	2,000-5,000	2	2
5 – 8	> 5,000	10	10
>8 – 9	2,000-5,000	3	3
>9	< 2,000	1	1

The derivation of appropriate default BMFs can only, at this stage, be considered as preliminary for use in screening of chemicals for the purposes of identifying those that need further scrutiny. In reviewing the appropriateness of the BMF applied in any particular assessment, it should be recognised that factors other than the log Kow and BCF should also be taken into account. Such factors should include the available evidence that may indicate a potential for the substance to metabolise or other evidence indicating a low potential for biomagnification. Evidence of a potential for significant metabolism may include:

- data from in vitro metabolism studies;
- data from mammalian metabolism studies;
- evidence of metabolism from structurally similar compounds;

- a measured BCF significantly lower than predicted from the log Kow, indicating possible metabolism.

Where evidence exists suggesting that such metabolism may occur, the BMF detailed above may be reduced. Where such reductions are proposed, a detailed justification must be provided.

Application of different spatial scales

Apart from the fact that for the assessment of the risks to the top predator an additional biomagnification factor is used the assessment also differs in terms of the input values that are used for the seawater concentrations that lead to the concentrations in the food of the different predators. For the first tier (or trophic level) of predators a worst-case assumption is that they obtain their prey equally from the local and regional area, respectively. This is in line with the assessment for freshwater and terrestrial organisms where a similar choice is made. For the calculation of the PECoral for the predators this implies the following:

$$PEC_{seawater} = 0.5 \cdot \left(PEClocal_{seawater,ann} + PECregional_{seawater} \right) \quad (91)$$

When $PEC_{seawater}$ is substituted in equation 89 this results in the following equation:

$$PEC_{oral,predator} = \left(PEClocal_{seawater,ann} + PECregional_{seawater} \right) \cdot 0.5 \cdot BCF_{fish} \cdot BMF_1 \quad (92)$$

Explanation of symbols

$PECoral_{predator}$	concentration in the food of the predator	$[mg \cdot kg^{-1}]$	
$PEC_{seawater}$	concentration in seawater	$[mg \cdot l^{-1}]$	
BCF_{fish}	bioconcentration factor	$[l \cdot kg^{-1}]$	eq. (73)
BMF_1	biomagnification factor in fish	[-]	Table 29
$PECregional_{seawater}$	predicted environmental concentration in the region	$[mg \cdot l^{-1}]$	
$PEClocal_{seawater,ann}$	annual average predicted environmental concentration	$[mg \cdot l^{-1}]$	

For the second tier of organisms, the top predators, it can be assumed that they obtain their prey mainly from the larger-scale regional marine environment which is to a lesser extent influenced by point source discharges. However, since it cannot be ruled out that certain top predators prey on organisms that receive their food from relatively small areas it is proposed to assume, as a realistic worst case, a 90/10 ratio between regional and local food intake. For the calculation of the oral intake rate for the top predator ($PECoral_{top\ predator}$) this implies:

$$PEC_{water} = 0.1 \cdot PEClocal_{seawater,ann} + 0.9 \cdot PECregional_{seawater} \quad (93)$$

When PEC_{water} is substituted in equation 90 this results in the following equation:

$$PEC_{oral,top-predator} = \left(0.1 \cdot PEClocal_{seawater,ann} + 0.9 \cdot PECregional_{seawater} \right) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2 \quad (94)$$

Derivation of the PNECoral values

In the derivation of the PNECoral values only toxicity studies reporting on dietary and oral exposure are relevant as the pathway for secondary poisoning refers exclusively to the uptake of chemicals through the food chain. However, reliable toxicity data for predatory marine birds (such as gulls and penguins) and mammals (such as seals, dolphins, whales and polar bears) are extremely limited (Nendza et al., 1997). Furthermore, testing of such species would be ethically unsound and contrary to animal welfare concerns. Therefore, it is necessary to extrapolate threshold levels for marine species from terrestrial species assuming there are interspecies correlations between laboratory bird species and marine predatory bird species, and between laboratory mammals (e.g. rats) and the considerably larger marine predatory mammals. This procedure is identical to that applicable for other media (see Section 3.8.3.5).

4.3.3.3 Testing strategy

If the PEC/PNEC ratio based on use of default BMF values indicates potential problems at any trophic level it should first be considered whether a refinement of the PEC-assessment is possible, i.e. the release and exposure assessment, including the fate related parameters such as determination of log Kow or BCF. In special cases it may even be considered to start with bioaccumulation studies in fish to determine the assimilation coefficient and the biological half-life of the substance (i.e. to determine BMF_1) prior to estimating or determining the bioconcentration factor (BCF). Also a refinement of the PNECoral could be considered, i.e. to require a long-term feeding study with laboratory mammals or birds to derive a more realistic NOECoral value. In conducting such a study according to current test methods, it may in special cases be considered whether to extend such studies to include satellite groups for determination of the concentration of the substance in the animals during exposure (i.e. to measure BMF_2 values). Alternatively or supplementary to actual testing can be monitoring of biota for which it is clear that they have lived in the environment that is covered in the assessment. Of course no active sampling of (top)predators should be performed, but for instance animals that are found dead can be used to get an indication about possible biomagnification factors in wildlife. Useful information might also be obtained from eggs or from biopsies of skin or blubber of marine birds or mammals.

4.4 PBT ASSESSMENT

4.4.1 Introduction

The PBT assessment is considered to be different from the local and regional assessment approaches, as it seeks to protect ecosystems where the risks are more difficult to estimate. These additional concerns for the marine environment, which may not be adequately addressed by the traditional risk assessment methodologies, can be summarised as:

a. the concern that hazardous substances may accumulate in parts of the marine environment and that:

   (i) the effects of such accumulation are unpredictable in the long-term;
   (ii) that such accumulation would be practically difficult to reverse;

b. the concern that remote areas of the oceans should remain untouched by hazardous substances resulting from human activity, and that the intrinsic value of pristine environments should be protected.

These concerns particularly occur with substances that can be shown both to persist for long periods and bioaccumulate in biota, and can give rise to toxic effects after a greater time and at a greater distance than chemicals without these properties. While this is also true for the freshwater environment, the additional concern in the marine environment is that once the chemical has entered the open seas, any cessation of emission will not necessarily result in a reduction in chemical concentration and hence any effects become difficult to reverse. Equally, because of the long-term exposures and long-life-cycle of many important marine species, effects may be difficult to detect at an early stage.

For PBT substances a "safe" concentration in the environment cannot be established with sufficient reliability. The PBT assessment is particularly developed to take into account the unacceptable high uncertainty in predicting reliable exposure and/or effect concentrations hampering quantitative risk assessment. The PBT assessment basically consists of two different steps:

- identification of PBT substances using specific criteria for the inherent properties; and
- an evaluation of the sources, major emissions and pathways to the marine environment to sufficiently establish the most appropriate and effective measures to reduce the releases to the marine environment.

The urgency and stringency of possible measures may, however, be dependent on the potential of the substance to be transported to the open sea. This can be assessed qualitatively by considering the use pattern, volumes and emissions or by using measured data. Open applications and wide dispersive uses of the substance are regarded particularly relevant as well as non-minimised direct discharges from production, formulation and industrial use.

4.4.2 PBT criteria

The criteria to be used to decide if a substance must be regarded as a PBT substance are summarised in **Table 30** below. The testing strategies to obtain the data that are necessary to decide whether a substance fulfils these criteria are given in separate sections on persistence, bioaccumulation and toxicity. The table contains two sets of criteria, one for PBT substances and a second category for so-called very persistent and very bioaccumulating substances (vPvB). This second category is developed under the recognition that for substances that are very persistent and bioaccumulate significantly in the food chain, high but unpredictable levels may be reached in wildlife or man over extended time periods. For such substances it is not necessary to demonstrate toxicity in laboratory testing as long-term effects can be anticipated anyway.

For most substances the available data will not allow to come to a definitive answer to the question if the substance must be considered under the PBT assessment. Hence screening data that identify whether the substance has a potential to be a PBT have to be made use of. The testing strategies in the following paragraphs should be followed and further information should be asked for accordingly. In deciding which information is requested (on P, B or T) care must be taken to avoid animal testing where possible. This implies that when for several properties further information is needed the assessment should be focussed on clarifying the potential for persistence first. When it is clear that the P criterion is fulfilled a stepwise approach should be followed to elucidate the B criterion, eventually followed by toxicity testing to clarify the T criterion.

Table 30 Criteria for identification of PBT and vPvB substances

Criterion	PBT criteria	vPvB-criteria
P	Half-life > 60 d in marine water or > 40 d in freshwater* or half-life > 180 d in marine sediment or > 120 d in freshwater sediment*	Half-life > 60 d in marine- or freshwater or >180 d in marine or freshwater sediment
B	BCF > 2,000	BCF > 5,000
T	Chronic NOEC < 0.01 mg/l or CMR or endocrine disrupting effects	Not applicable

* For the purpose of marine environmental risk assessment half-life data in freshwater and freshwater sediment can be overruled by data obtained under marine conditions.

In principle, substances are selected when they fulfil the criteria for all three inherent properties P, B and T. However, certain flexibility is required in their application for instance in cases where one criterion is marginally not fulfilled but the others are exceeded considerably. This may include for example substances that do not fulfil the persistence criteria but bioaccumulate significantly and are measured in marine biota distant from anthropogenic sources.

It is realized that the individual trigger values may be scientifically disputable when considered in isolation. However, by applying the *combined set of criteria* it is expected that substances will be selected for which quantification of the risk by using the PEC/PNEC approach is considered too uncertain.

The PBT assessment has links to similar concepts discussed in other fora (e.g. the UNEP Stockholm Convention on Persistent Organic Pollutants, the OSPAR Hazardous Substances Strategy (OSPAR, 1998)). The discussions from the other fora have been carefully considered.

4.4.3 Testing strategy for the P criterion

4.4.3.1 Introduction

The persistence of a substance reflects the potential for long-term exposure of organisms but also the potential for the substance to reach the marine environment and to be transported to remote areas. The assessment of the (potential for) persistency in the marine environment should in principle be based on actual half-life data determined under marine environmental conditions. Depending on whether a substance has a half-life smaller or greater than the cut-off criterion it is decided if a substance fulfils the P criterion. When these key data are not available other types of available information on the degradability of a substance can be used to decide if further testing is needed to assess the potential persistence. In this approach three different levels of information are defined according to their perceived relevance to the criteria:

- experimental data on persistence in the marine environment;
- other experimental data;
- data from biodegradation estimation models.

An explanation on what type of information is relevant within these levels and the relevant cut-off values is given below. It must be noted that this approach reflects existing knowledge on biodegradation and should be considered as a pragmatic approach to make optimal use of the available data and methods. Clearly, more research is needed to better estimate the persistence in the marine environment from existing biodegradation tests. Moreover, other degradation

mechanisms such as hydrolysis and photolysis should be taken into account where they can be shown to be relevant.

4.4.3.2 Experimental data on persistence in the marine environment

In principle the persistence in the marine environment should be assessed in simulation test systems that determine the half-life under relevant environmental conditions. The determination of the half-life should include assessment of metabolites with PBT-characteristics. The half-life should be used as the first and main criterion in order to determine whether substances should be regarded as persistent. Hence appropriate half-life data from valid simulation tests override data from the other levels of information. Substances with a half-life in marine water of > 60 days or a half-life of >180 days in marine sediment are considered as being persistent. Substances are considered very persistent (vP) when the half-life in marine or freshwater is > 60 days or the half-life in marine or freshwater sediments is > 180 days.

Recommended simulation test methods for water and sediment are described in Section 4.2.3.3.

Tests performed under marine conditions should use media from marine areas not directly influenced by freshwater outlets or runoffs. This means that samples taken for inoculation and conduction of marine biodegradation simulation tests must not contain significant amounts of freshwater microorganisms as these to a larger extent could already have been pre-exposed or adapted to the substance. It is not possible to establish specific criteria and each test must be evaluated case-by-case. However, the content of freshwater in the sample should be low (i.e. a large dilution as e.g. determined by salinity), the sample should be taken from the water column (and not the surface), the content of microorganisms should be low (compared to freshwater) and cross-contamination during handling, transport and testing should be avoided.

4.4.3.3 Other experimental data

In case no half-life data are available for marine water or sediment the decision whether a substance is potentially persistent needs to be based on other experimental data. If available, use can be made of the half-life values from simulation tests of degradation in freshwater. Since the degradation in marine waters other than estuaries is expected to be slower than in freshwater a criterion of >40 days for freshwater and >120 days for freshwater sediments has to be used.

Where no data are available which allow the assignment of a degradation half-life in the environment based on simulation test data, other experimental data may be considered. The available information relating to biodegradability is dominated by test results on Ready Biodegradability (EU Annex V C.4 A, C, E and F; OECD guidelines 301A-D, 1992f, 306, 1992e or equivalent) and to a lesser extent by data on the Inherent Biodegradability (EU Annex V C.12 and C.9; OECD TG A-C, 1981d or equivalent). The conditions for degradation in the marine environment are far from the conditions applied in these standard tests (cf. Section 4.2.3). Hence, extrapolation of the existing biodegradation information (either measured data from ready and inherent tests or results from QSAR modelling) to degradation rates in the marine environment is very difficult and care should be taken not to over-interpret the outcome of such tests. However, in order to use the available information to select potentially persistent substances, this information should be used in the following way:

- readily biodegradable substances (fulfilling or not fulfilling the 10-day window criterion) are considered as not persistent in the PBT assessment;

- when a substance does not fulfil the criteria for ready biodegradability as defined in sections on biodegradation and for the marine ready test (see Sections 2.3.6 and 4.2.3.4), it is considered as being potentially persistent. The 10-day window criterion should not be used here as an additional criterion. If the substance fulfils the criteria for B and T, further testing is needed. It must be noted that in this case it is not considered appropriate to perform inherent biodegradability tests but rather to go directly to simulation testing;
- when results are available showing that a substance does not fulfil the criteria for inherent biodegradability as defined within the Annex V method or the OECD guideline this is a clear indication that the substance will not biodegrade in the marine environment either. The substance will be regarded as potentially persistent. When the (screening) criteria for B and T are also fulfilled, further testing is needed in order to determine the half-life in the environment.
- when a substance passes the criteria for inherent biodegradability tests this does not necessarily indicate that it will not be persistent under environmental conditions. However, in order to make the best use of available information it is accepted to use the results of two specific tests when they fulfil certain criteria as an indication that the substance is not persistent. These test are:
  - Zahn-Wellens Test (EU Annex V C.9, OECD 302B, 1992g): Pass level (70% mineralisation) must be reached within 7 days, log-phase should be no longer than 3 days, percentage removal in the test before degradation occurs should be below 15%, not tested with pre-adapted microorganisms;
  - MITI II -test (OECD 302C, 1981d): Pass level must be reached within 14 days; log-phase should be no longer than 3 days, not tested with pre-adapted microorganisms.

In case a range of biodegradation data, including conflicting data, is available, a case-by-case assessment is needed, using a weight of evidence approach, in order to decide whether a substance has the potential to be persistent (see also Section 2.3.6).

4.4.3.4 Data from biodegradation estimation models

For new substances, priority existing substances and biocides, information from a ready biodegradability test is normally available and therefore an initial decision whether the substance is potentially persistent can be taken. However, for many other substances no data will be available or the available information is difficult to interpret. For these substances it can be helpful to apply models that estimate the potential for biodegradation in the environment.

In a preliminary assessment whether a substance has a potential for persistence in the marine environment and hence for asking for actual test data it is proposed to consider use of the BIOWIN program. This program estimates aerobic biodegradability of organic chemicals using 6 different models:

1. linear model,
2. non-linear model,
3. ultimate biodegradability timeframe model,
4. primary biodegradability timeframe model,
5. MITI linear model,
6. MITI non-linear model;

The use of the results of these programs in a conservative way may fulfil the needs for evaluating the potential for persistency. The use of three out of the six models is suggested as follows:

- non-linear model prediction: does not biodegrade fast (<0.5) **or**
- MITI non-linear model prediction: not readily degradable (<0.5) **and**
- ultimate biodegradation timeframe prediction: ≥ months (<2.2)

When predictions of these three models are combined relatively few not readily biodegradable substances will not be identified, without in the same time causing a significant increase in the number of falsely included readily biodegradable substances.

The preliminary character of this method to identify potentially persistent substances in the marine environment is emphasised, and further possible development of a suitable methodology is recommended. The BIOWIN program is available from the US EPA's internet site (http://www.epa.gov/oppt/exposure/docs/episuitedl.htm).

4.4.3.5 Summary of the P assessment

A summary of the assessment of biodegradation data in the context of the P criterion is given in **Table 31** below.

Table 31 Overview of P-assignment for different types of biodegradation data

Type of data	Criterion	Definitive assignment	Screening assignment [1]
DT50 marine water	> 60 d	VP	-
DT50 freshwater [2]	> 40 d	P [3]	-
	> 60 d	VP	-
DT50 marine sediment	> 180 d	VP	-
DT50 freshwater sediment [2]	> 120 d	P [3]	-
	> 180 d	VP	-
Readily biodegradable [4]	Yes	Not P	-
	No	-	P or vP
Inherently degradable	Yes	Not P [5]	-
	No	-	P or vP
QSAR	Non-linear model prediction < 0.5 or MITI non-linear model prediction < 0.5 and Ultimate biodegradation timeframe prediction < 2.2	-	P or vP

1) These screening methods give an "open-ended" categorisation of the substance as either being potentially P or vP, which cannot easily be related to a half-life for biodegradation.
2) Data for estuaries should also be considered in this category.
3) Half-life data in freshwater and freshwater sediment can be overruled by data obtained under marine conditions.
4) Regardless of whether the 10-d window criterion is fulfilled.
5) This only applies to cases where the specific criteria as mentioned in Section 4.4.3.3 are fulfilled.

4.4.4 Testing strategy for the B criterion

4.4.4.1 Introduction

Substances can accumulate in aquatic organisms directly from the water, i.e. bioconcentration, or via uptake through the foodchain, i.e. biomagnification. A high bioaccumulation potential of a substance is of particular concern for the marine environment due to the possible accumulation in the foodchains and the potential long-term effects that may occur in organisms at the top of these foodchains. Whereas different models and parameters are available to evaluate bioconcentration for organic chemicals, suitable parameters to evaluate accumulation in marine foodchains are not available. The bioconcentration factor (BCF) in aquatic organisms is traditionally used as a first indicator for bioaccumulation (see Section 3.8.2).

In principle, the assessment of the (potential for) bioaccumulation in the context of the PBT assessment makes use of measured bioconcentration factors in marine or freshwater organisms. Where these are not available BCF values may be estimated from the octanol/water partition coefficient (Kow) using QSAR models. In addition, Kow values, either experimentally determined or estimated can be used directly to assess the potential for bioaccumulation.

4.4.4.2 Assessment of measured BCF data

The decision whether or not a substance fulfils the B criterion should in principle be based on measured data on bioconcentration in aquatic species. Data from freshwater as well as marine species can be used. Extensive guidance on the quality assessment of such data can be found elsewhere (e.g. OECD, 2001c). A substance is considered to fulfil the B criterion when the measured BCF on a wet weight basis exceeds a value of 2,000. A substance is considered very bioaccumulative (vB) when the BCF exceeds a value of 5,000.

4.4.4.3 Assessment of the potential for bioaccumulation

When measured BCF values are not available the Kow or the BCF based on modelling can be used to indicate the liability to bioaccumulate from water. For substances with log Kow < 6 assessment on the basis of Kow or estimated BCF does not make a real difference since all available BCF models are linear (see Section 3.8.3.2). The B criterion for log Kow is therefore directly derived from this linear relationship. A substance is considered to potentially fulfil the B criterion when log Kow exceeds a value of 4.5.

For highly hydrophobic substances, e.g. with log Kow > 6, experimentally derived BCF values tend to decrease with increasing log Kow. Several conceptual explanations as well as explanations referring to experimental artefacts can be given for this decline. For these substances the available BCF models can lead to very different results. As a consequence the potential for bioaccumulation is assessed by expert judgement on the basis of the log Kow value and the estimated BCF using the available BCF models. Such an assessment must be done on a case-by-case basis taking into account what is known about the BCF QSAR-models and the specific properties of the substance, in particular what is known to affect uptake and the potential for metabolism in aquatic organisms. Care must be taken that substances with high log Kow values are not deleted from selection processes without applying expert judgement to them.

It must be noted that for priority existing substances, new substances and biocides a measured octanol/water partition coefficient is usually available. Additionally a range of QSAR models can be used to estimate this parameter (see e.g. Chapter 4, Meylan et al., 1999; OECD, 2001c).

4.4.4.4 Other information relevant for assessment of the B criterion

In addition to the above-mentioned data on bioconcentration or bioaccumulation in aquatic species evidence that a substance shows high bioaccumulation in other species may also be used to decide whether the B criterion is fulfilled. Such evidence may be based on information from specific laboratory tests or from field studies. Specific attention needs to be paid to measured data in biota. Measured data in biota are a clear indicator that a substance is taken up by an organism. However, they are not an indicator that significant bioconcentration or bioaccumulation has occurred. The interpretation of such data in terms of actual bioaccumulation or biomagnification factors can especially be difficult when the sources and levels of the exposure (through water as well as through food) are not known or cannot be estimated reasonably.

4.4.5 Testing strategy for the T criterion

4.4.5.1 Introduction

For persistent and bioaccumulative substances long-term exposure can be anticipated and expected to cover the whole life-time of an organism and even multiple generations. Therefore chronic or long-term ecotoxicity data, ideally covering the reproductive stages should in principle be used for the assessment of the T criterion. In practice, however, the principal data available for most chemicals will be for short-term effects, and this must, in the first instance, be used to drive initial selection. Mammalian toxicity data must also be considered in the selection due to the fact that toxic effects on top predators, including man may occur through long-term exposure via the food-chain. The selection criteria should therefore consider two types of effect data, either of which will trigger selection.

4.4.5.2 Chronic effects data

A substance is considered to fulfil the toxicity criterion when:

- the long-term NOEC for marine or freshwater organisms is less than 0.01 mg/l. When other information is available such as data on sediment toxicity or data from feeding studies this needs to be assessed on case-by-case basis. For biocides and pesticides results from sub-chronic, chronic or reproduction avian toxicity tests may be available. A chronic NOEC of less than 30 mg/kg/food can be used as a criterion.

or

- when the substance is classified as Carcinogenic, (category 1 & 2), Mutagenic (category 1 & 2) or Toxic for Reproduction (category 1, 2 & 3) or when there is evidence of chronic toxicity, as identified by the classifications T, R45, R46, R48, R60 and R61 or Xn, R48, R62, R63 and R64 [8].
- when a substance is classified as Carcinogenic category 3 or Mutagenic category 3 a case-by-case assessment must be carried out to decide whether the evidence is sufficient for the substance to be considered as toxic, in the context of this PBT assessment, or whether further information is needed to clarify this potential concern.

or

- when there is substantiated evidence of long-term toxicity (e.g. endocrine disrupting effects). Such evidence needs to be considered on a case-by-case basis.

4.4.5.3 Acute effects data (screening level)

Where data on chronic effects are not available short-term toxicity data for marine or freshwater organisms can be used to determine whether a substance is a potential PBT provided the screening criteria for P and B are fulfilled. In the context of the PBT assessment a substance is considered to be potentially toxic when the L(E)C50 to aquatic organisms is less than 0.1 mg/l. If a substance is confirmed to fulfil the ultimate P and B criteria chronic toxicity data are

[8] In relation to the use of R64 in the context of the PBT assessment care should be taken that the actual assignment of the R-phrase is a result of results of one or two generation studies in animals which indicate the presence of adverse effects on the offspring due to transfer in the milk (see Annex VI to Directive 67/548).

required to deselect this substance from being considered as a PBT. In principle chronic toxicity data, when obtained for the same species, should override the results from the acute tests.

In the context of the PBT assessment acute mammalian toxicity tests are normally not considered to provide an appropriate indication of chronic effects. However, it should be noted that when a substance is classified as Very Toxic or Toxic after oral dosing (LD50 < 200 mg/kg bw/d) and the toxicity is expected to be the result of systemic effects, the probability that the chronic NOAEL after repeated dosing (e.g. 28 d or 90 d) will be less than the trigger value for R48 (± 150 or 50 mg/kg bw/d, respectively) will be high. The substance would therefore be classified and considered as fulfilling the T criterion. In that case verification of the actual chronic toxicity by performing animal testing is not recommended. When the P and B screening criteria are also fulfilled the substance can be considered as a PBT unless additional information indicates otherwise.

4.4.5.4 Estimated effects data

In case where no acute or chronic toxicity data are available the assessment of the T criterion at a screening level can be performed using data obtained from quantitative structure activity relationships (QSARs). Guidance on the use of QSARs for specific groups of substances can be found in Chapter 4.

It must be noted that since long-term effects can be anticipated for very bioaccumulative substances (vPvB), further animal testing for such substances is deemed unnecessary.

5 RISK CHARACTERISATION

5.1 INTRODUCTION

Having conducted the exposure assessment and the dose (concentration) - response (effect) assessment for all environmental compartments, either a quantitative risk characterisation or a qualitative risk characterisation is carried out.

The quantitative risk characterisation is carried out by comparing the PEC with the PNEC. This is done separately for each of the environmental compartments identified in Section 1.2 and **Tables 1 and 2**:

Inland environmental compartments:

- aquatic ecosystem;
- terrestrial ecosystem;
- atmosphere;
- top predators;
- microorganisms in sewage treatment plants.

Marine environmental compartments:

- aquatic ecosystem;
- top predators.

A list of the different PEC/PNEC ratios that should be considered for the inland and marine environments is given in **Tables 32 and 33**, respectively. Depending on whether the risk characterisation is performed for a new substance, for an existing substance or for a biocidal active substance, different conclusions can be drawn on the basis of the PEC/PNEC ratio for the different endpoints, and different strategies can be followed when PEC/PNEC ratios greater than one are observed. Therefore, the descriptions of the risk characterisation approaches are given separately for new substances, for existing substances and for biocides. However, a number of general premises apply to the procedures that have to be followed. These are given first.

Table 32 Overview of PEC/PNEC ratios considered for inland risk assessment *

Local	Regional
$PEClocal_{water}/PNEC_{water}$	$PECregional_{water}/PNEC_{water}$
$PEClocal_{sediment}/PNEC_{sediment}$	$PECregional_{sediment}/PNEC_{sediment}$
$PEClocal_{soil}/PNEC_{soil}$	$PECregional_{agr.soil}/PNEC_{soil}$
$PEC_{stp}/PNEC_{microorganisms}$	
$(0.5 \cdot PEClocal,oral_{fish} + 0.5 \cdot PECregional,oral_{fish})/PNECoral$	
$(0.5 \cdot PEClocal,oral_{worm} + 0.5 \cdot PECregional,oral_{worm})/PNECoral$	

* It has to be noted that these ratios have to be derived for all stages of the life-cycle of a compound.

Table 33 Overview of PEC/PNEC ratios considered for marine risk assessment *

Local	Regional
$PEClocal_{seawater}/PNEC_{saltwater}$	$PECregional_{seawater}/PNEC_{saltwater}$
$PEClocal_{sediment}/PNEC_{marine\ sediment}$	$PECregional_{sediment}/PNEC_{marine\ sediment}$
$[(PEClocal_{seawater,ann} + PECregional_{seawater}) \cdot 0.5 \cdot BCF_{fish} \cdot BMF_1]/PNECoral_{predator}$	
$[(0.1 \cdot PEClocal_{seawater,ann} + 0.9 \cdot PECregional_{seawater}) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2]/PNECoral_{top\ predator}$	

* It has to be noted that these ratios have to be derived for all stages of the life-cycle of a compound.

When no quantitative risk characterisation can be carried out, for example for remote marine areas or when either PEC or PNEC cannot be properly derived, a qualitative risk characterisation should be conducted. This is described in Section 5.6.

5.2 GENERAL PREMISES FOR RISK CHARACTERISATION

In general, the risk characterisation phase is carried out along the following steps (see **Figure 17**):

- determine the PEC/PNEC ratios for the different environmental compartments considered.

Dependent on these PEC/PNEC ratios:

- determine whether further information/testing may lead to a revision of these ratios;
- ask for further information/testing when appropriate;
- refine the PEC/PNEC ratio.

This iterative process should be continued until a final conclusion regarding the environmental risks can be reached.

For the risk characterisation for the aquatic and terrestrial ecosystems, including secondary poisoning, a direct comparison of the PEC and PNEC values is carried out, presuming that the relevant data are available. If the PEC/PNEC ratio is greater than one the substance is "of concern" and further action has to be taken.

For the air compartment usually only a qualitative assessment of abiotic effects is carried out. If there are indications that one or more of these effects occur for a given substance, expert knowledge should be consulted or the substance be handed over to the relevant international group, e.g. to the responsible body in the United Nations Environment Programme (UNEP) for ozone depleting substances. In some cases also an assessment of the biotic effects to plants can be carried out.

The risk characterisation for top predators is made by comparing the PECoral with the PNECoral in accordance with the procedure described in Sections 3.8 and 4.3.3. If the ratio PECoral / PNECoral is greater than one and a refinement of the PECoral or the PNECoral is not possible or reasonable, risk reduction measures should be considered.

The risk characterisation for microorganisms in sewage treatment systems is done by comparing the PEC_{stp} with the $PNEC_{microorganisms}$. If the ratio of these two values is greater than one, this indicates that the substance may have a detrimental effect on the function of the STP and therefore is "of concern".

When PEC/PNEC ratios greater than one have been calculated, the competent authority should consult industry in order to see if additional data on exposure and/or ecotoxicity can be obtained in order to refine the assessment.

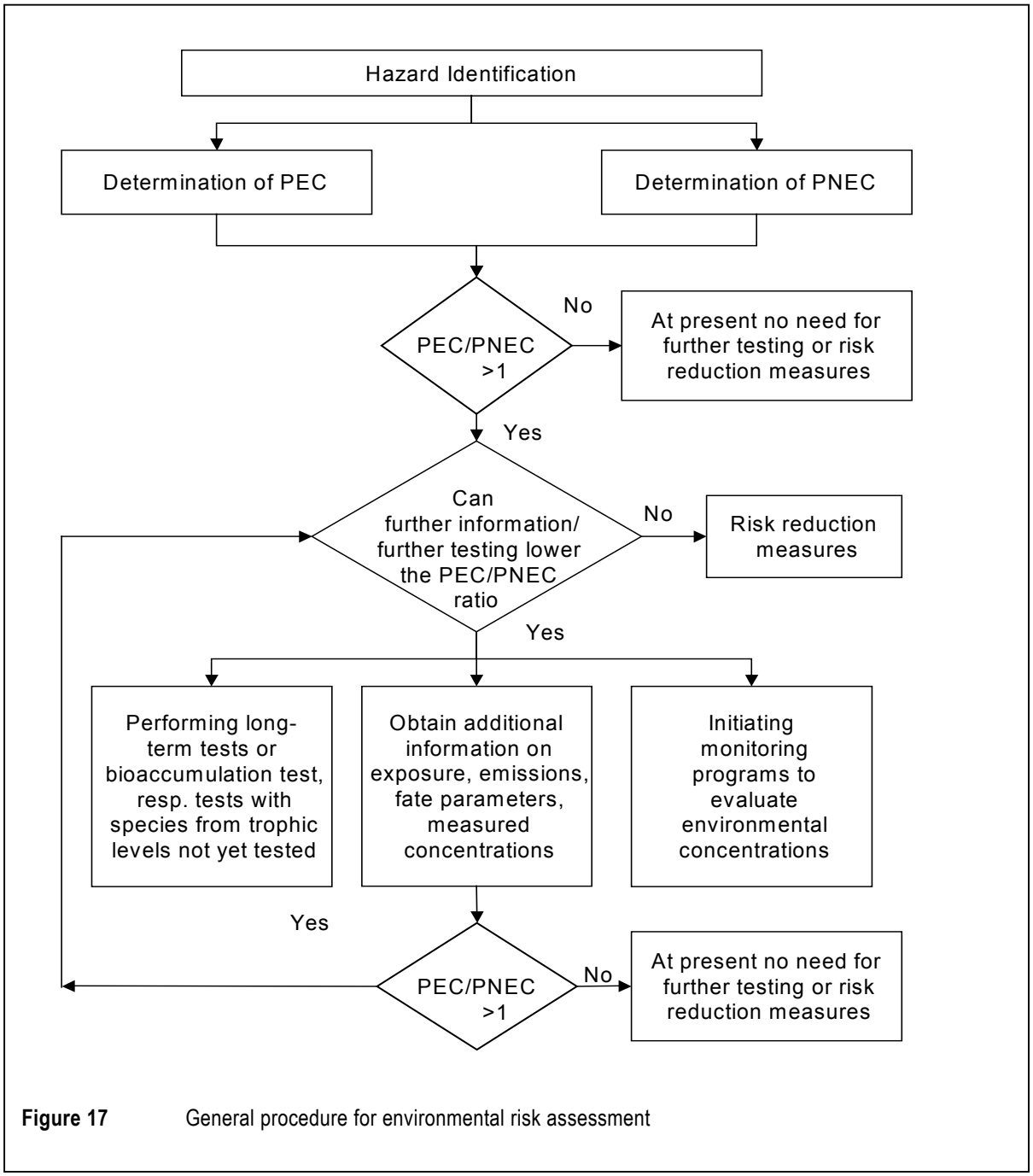

Figure 17 General procedure for environmental risk assessment

Dependent on the value of the PEC/PNEC ratio, there may be cases where, assuming realistic PEC values which cannot be further refined (e.g. representative monitoring data), any further testing which lowers the assessment factor cannot decrease the PEC/PNEC ratio below one. In that case, no further testing should be required and the substance in question should be a candidate for risk reduction.

If a refinement of the risk characterisation is possible but the necessary data are not available, further information and/or testing needs to be requested. On a case-by-case basis, a decision must be taken as to whether both the PEC and PNEC will be revised or only one of them. Consideration should be given to which of the parameters that will be most sensitive to revision as a result of further testing. The decision by the competent authority to request additional data should be transparent and justified and should be based on the principles of lowest cost and effort, highest gain of information and the avoidance of unnecessary testing on animals. This iterative approach has precautionary aspects as data gaps are filled by worst-case assumptions or high assessment factors. Guidance on which tests to conduct and how the results of such tests can be used to revise the PEC and/or the PNEC is given in Sections 6.2 and 6.3 of this document. Detailed guidance on how to use (Q)SARs in order to clarify whether further testing is necessary, and how these (Q)SARs can assist in deciding on the testing strategy, is given in Chapter 4 (Use of QSARs).

5.3 RISK CHARACTERISATION FOR EXISTING SUBSTANCES

The environmental risk assessment in the context of article 5 and Annex 3 of Regulation 1488/94 involves the comparison of the PEC and PNEC values for the different endpoints mentioned above. Regulation 793/93 mentions three different conclusions that may apply on the basis of the risk characterisation:

Conclusion (i)	There is need for further information and/or testing;
Conclusion (ii)	There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already;
Conclusion (iii)	There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

The general scheme given in **Figure 17** applies for the risk characterisation of existing substances. At the first comparison of the PEC and PNEC values it is assumed that industry is contacted and that all available information is used to derive these. If the PEC/PNEC ratio is found to be less than or equal to one for each compartment, conclusion (ii) shall apply. If the PEC/PNEC ratio for any compartment is greater than one, the rapporteur shall judge whether further information and/or testing are required to clarify the concern (conclusion (i)) or if (further) risk reduction measures are necessary (conclusion (iii)). The judgement shall be carried out on the basis of the size of the PEC/PNEC ratio and some additional indicators such as:

1. indications of bioaccumulation potential;
2. the shape of the toxicity/time curve in ecotoxicity testing;
3. indications of other adverse effects on the basis of toxicity studies, e.g. classification as a mutagen, toxic or very toxic or as harmful with a risk phrase R40 (“Possible risk of irreversible effects”) or R48 (“Danger of serious damage to health by prolonged exposure”);
4. data on structurally analogous substances.

Furthermore indications of other adverse effects, e.g. classification with the risk phrases R45 (“May cause cancer”), R46 (“May cause heritable genetic damage”), R47 (“May cause birth defects”) and R60 (“May impair fertility”) may be considered as well.

These factors especially pertain to substances for which a “standard” risk assessment cannot be performed, for instance because the models that are applied are not suitable, or for substances for which the standard data set does not give suitable information on the properties of the substance (for instance highly hydrophobic substances that do not show any toxicity in short-term tests).

A specific risk characterisation is made for secondary poisoning. PECoral and PNECoral are calculated according to the procedures described in Section 3.8, either by using the available BCF values or by calculation of BCF from the octanol/water partition coefficient. Both the local and the regional PEC_{water} are used to calculate PECoral.

5.4 RISK CHARACTERISATION FOR NEW SUBSTANCES

The risk characterisation in the context of article 5 of and Annex III to Directive 93/67 also involves the iterative revision of the PEC/PNEC ratio as a function of the degree of risk predicted. In addition, a link is made with the tonnage triggers for further testing as laid down in Article 7.2 of Directive 67/548. If the PEC/PNEC ratio is found to be less than or equal to one, the conclusion laid down in Article 3(4)(i) of the Directive shall apply:

- the substance is of no immediate concern and need not to be considered again until further information is made available in accordance with Articles 7(2), 8(3), 8(4) or 14(1) of the parent Directive 67/548.

If the PEC/PNEC ratio is greater than one, the authority should judge which of the conclusions set out in Article 3.4(ii), 3.4(iii) or 3.4(iv) that shall apply:

- the substance is of concern and the competent authorities shall decide what further information is required for revision of the assessment but shall defer a request for that information until the quantity placed on the market reaches the next tonnage threshold as indicated in Article 7(2), 8(3) or 8(4) of Directive 67/548;
- the substance is of concern and further information shall be requested immediately;
- the substance is of concern and the competent authority shall immediately make recommendations for risk reduction.

In the light of rather extensive experience of testing and evaluation procedures linked with the aquatic environment, it has been possible to develop a relatively structured decision scheme in relation to the aquatic compartment. This scheme is given in **Figure 18**.

It is assumed that for substances entering the scheme, data equivalent to those foreseen in Annex VII A (the base set) to Directive 67/548 will be available. Information contained in the base set is used to estimate the PEC and the PNEC for the aquatic environment. Furthermore, the assumption is made in the decision scheme that where the PEC/PNEC ratio exceeds one, the authority has discussed this situation with the notifier and that the values, in particular the PEC, have already been amended in the light of further information provided by the notifier. The first PEC/PNEC ratio referred to in **Figure 18** is therefore the value as amended after further discussions with the notifier.

Depending on the value of the PEC/PNEC ratio, one of the options available under article 3.4 of Directive 93/67 is chosen. Where the PEC/PNEC ratio is between 10 and 100, the decision whether to request further testing immediately or at the 10 tonnes per annum production level will be made on the basis of a number of factors including:

1. indications of bioaccumulation potential;
2. the shape of the toxicity/time curve in ecotoxicity testing;
3. data on structurally analogous substances.

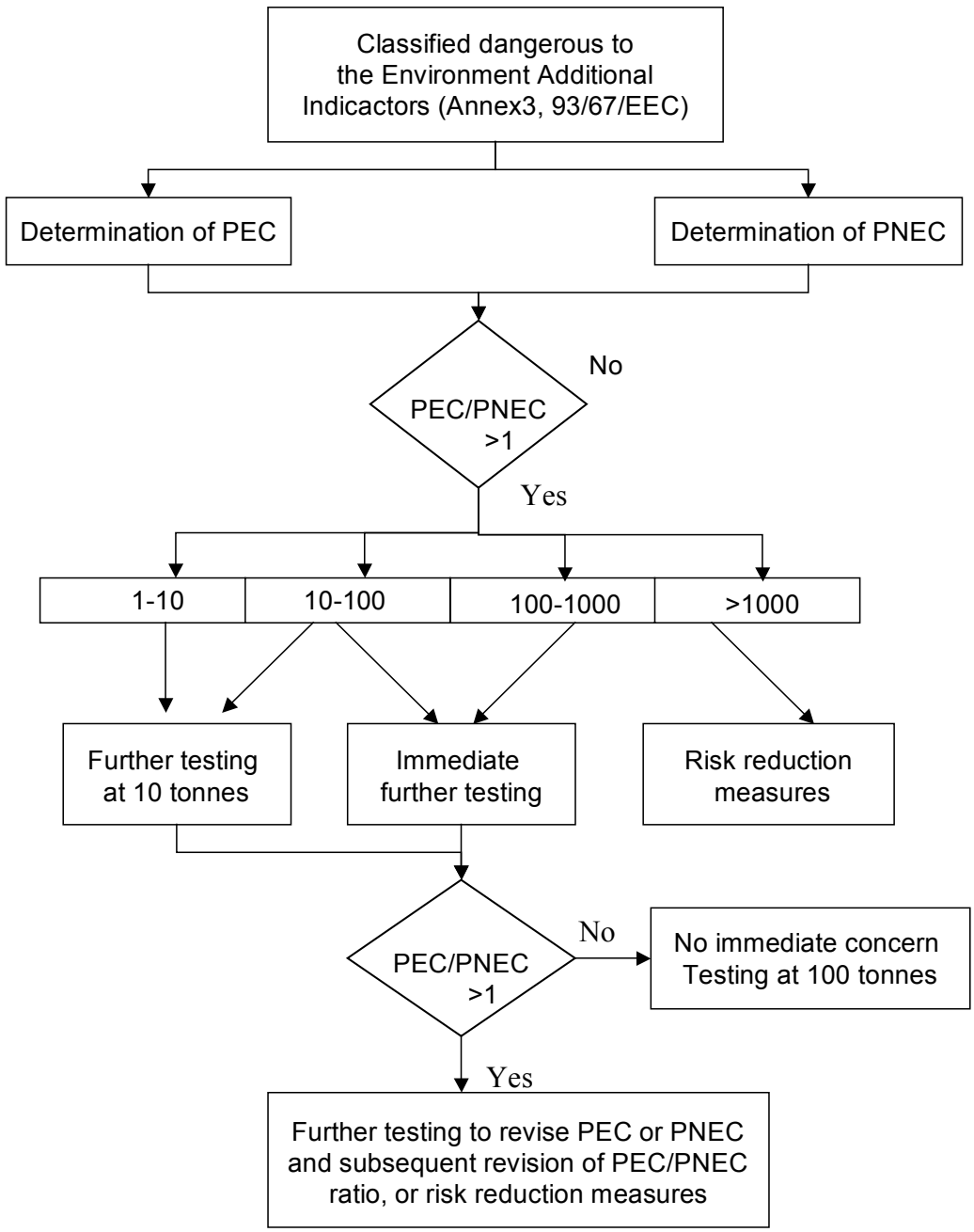

Figure 18 Decision scheme for aquatic risk characterisation of new chemicals

The factor "indications of other adverse effects on the basis of toxicity studies, e.g. classification as a mutagen, as toxic or very toxic or as harmful with risk phrase R40 ("Possible risk of irreversible effects") or R48 ("Danger of serious damage to health by prolonged exposure")" can be used to decide whether a substance will enter the scheme; so whether a risk assessment should be performed. This factor cannot be used to decide whether further testing is needed.

The base set testing package (Annex VII A) of the Directive generates relatively little data which are of relevance to the terrestrial and atmospheric compartments: further but nevertheless still limited data are foreseen at level 1 and level 2 (Annex VIII). Where consideration of either of these two compartments is of relevance to the environmental risk assessment of a particular substance, further testing and progressive revision of the PEC/PNEC should be carried out on a case-by-case basis in the light of the guidance set out in Section 6.

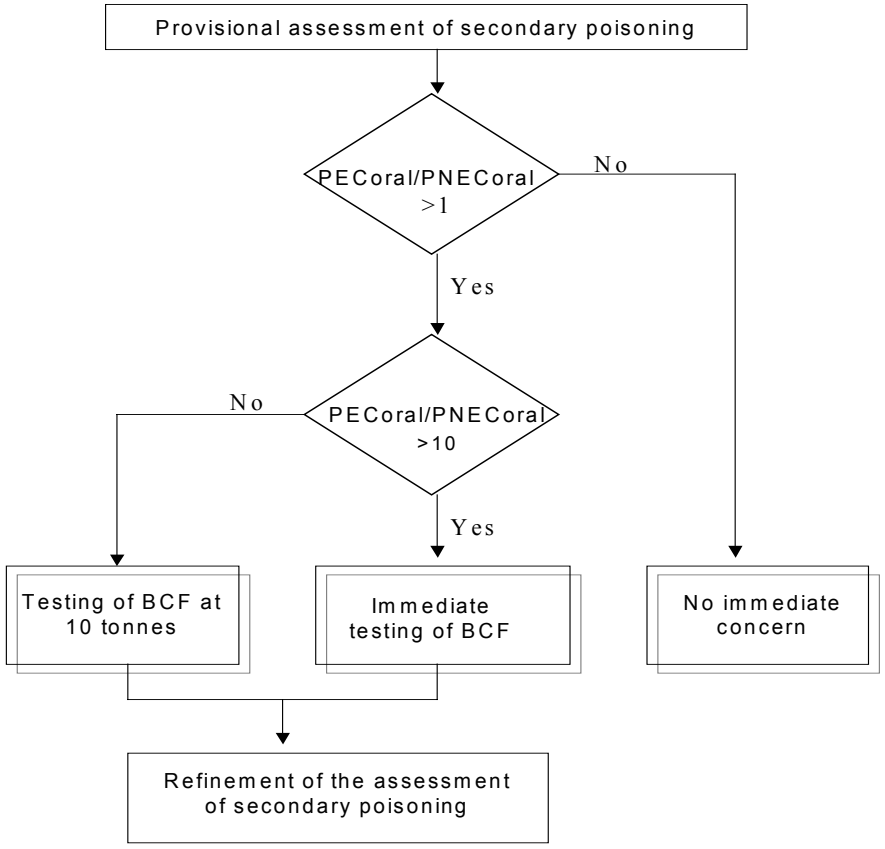

Figure 19 Decision scheme for risk characterisation for secondary poisoning for new chemicals

For the risk characterisation for top predators a specific assessment scheme applies. This scheme is given in **Figure 19**. In this case the yearly average PEClocal for water is used to calculate PECoral. Based on the results of the provisional assessment of secondary poisoning where a calculated BCF value is used (see Section 3.8), it is decided whether or not a bioaccumulation test should be requested, either immediately or at the 10 tonnes per annum production level. It should be noted that a bioaccumulation test is a level 1 test. The result of the bioaccumulation test is used to refine the risk characterisation for top predators. If the ratio of PECoral and PNECoral is still greater than one, secondary poisoning could be a critical pathway for fish-

eaters. This may lead to a request for more specific tests, for instance long-term dietary studies on birds, that can be used to facilitate a better calculation.

5.5 RISK CHARACTERISATION FOR BIOCIDES

The environmental risk characterisation for biocidal active substances in the context of Article 5 and Annex VI of Directive 98/8 involves i.a. the comparison of PEC and PNEC values for relevant environmental compartments as well as for non-target organisms. According to Articles 10 and 11 of the Directive, the possible results of the risk assessment are:

- there is a need for further information and/or testing;
- the substance has unacceptable effects on the environment and consequently, it cannot be included in Annex I, IA or IB;
- the substance may be considered for inclusion in Annex I, IA or IB of the Directive.

The decision on inclusion in Annex I, IA or IB of the Directive also depends on other criteria regarding, e.g., other unacceptable effects and efficacy (cf. Directive 98/8 and the Technical Notes for Guidance on Annex I inclusion). The inclusion may, where appropriate, be subject to certain requirements and conditions for use. When it is concluded that the active biocidal substance can be included in Annex I, IA or IB, the inclusion may be granted for an initial period not exceeding 10 years (Article 10 of Directive 98/8). The inclusion of an active substance may be renewed on one or more occasions for periods not exceeding 10 years.

Additional to these main conclusions, some substances included in Annex I, IA or IB may be candidates for a future comparative assessment (Article 10 of Directive 98/8). This may be the case when the PEC/PNEC ratio is > 0.1 and ≤ 1 (cf. the Technical Notes for Guidance (TNsG) on Annex I inclusion, 2001).

It is considered an unacceptable effect if PEC/PNEC > 1 for non-target organisms and aquatic organisms, or if the bioconcentration factor (BCF) > 1 related to fat tissues in non-target vertebrates, if BCF for aquatic organisms > 1000 for readily biodegradable substances or if BCF for aquatic organisms > 100 for not readily biodegradable substances (cf. Annex VI to Directive 98/8).

If the PEC/PNEC ratio is > 1 the Member State shall judge, on the basis of the size of that ratio and on other relevant factors, if further information and/or testing are required to clarify the concern, if risk reduction measures are necessary or if the substance cannot be included in Annex I, IA or IB at all.

Finally, if a quantitative risk characterisation cannot be conducted, a qualitative risk characterisation should be conducted, cf. below.

5.6 QUALITATIVE RISK CHARACTERISATION

Although the use of quantitative PEC/PNEC ratios is the preferred procedure for carrying out an environmental risk assessment, there may be cases where a quantitative risk characterisation cannot be carried out. This is, e.g., the case for assessment of risks for remote marine areas and for substances where either PEC or PNEC cannot be properly calculated. In these cases, the risk characterisation shall entail a qualitative evaluation of the likelihood that an effect will occur under the expected conditions of exposure (see Annex III, par. 4.2 of Directive 93/67).

For a qualitative assessment of risks for remote marine areas, the PBT approach should be used. Substances fulfilling the PBT criteria regarding Persistence, Bioaccumulation and Toxicity (cf. Section 4.4) are of priority for further risk management consideration. For such substances, an evaluation of the sources, major emissions and pathways to the marine environment should take place in order to sufficiently establish the most appropriate and effective measures to reduce the releases to the marine environment.

If no PEC can be properly calculated and a qualitative exposure assessment indicates that no environmental compartment is likely to be polluted, the substance should be automatically set aside as of no immediate concern. However, if a qualitative exposure assessment indicates that environmental exposure is likely, the risk characterisation will entail consideration of the special factors mentioned in Sections 5.3 and 5.4. Depending on which and how many of those factors that apply, a decision should be made on which of the options set out in Article 3.4 of Directive 93/67 or Article 5 of Regulation 1488/94 that is applicable.

For some substances it may not be possible to undertake a full quantitative risk assessment, using a $PEC_{water}/PNEC_{water}$ ratio because of the inability to calculate a $PNEC_{water}$. This can occur when no effects are observed in short-term tests. However, an absence of short-term toxicity does not necessarily mean that a substance has no long-term toxicity, particularly when it has low water solubility and/or high hydrophobicity. For such substances, the concentration in water (at the solubility limit) may not be sufficient to cause short-term effects because the time to reach a steady-state between the organism and the water is longer than the test duration.

For these substances, therefore, it is recommended to conduct a qualitative risk assessment in order to decide if further long-term testing is required. Such an assessment should take full account of the level of exposure (PEClocal or PECregional, as appropriate) as well as of the probability that long-term effects may occur despite the absence of short-term effects. Thus, especially for non-polar organic substances with a potential to bioaccumulate (log Kow > 3), the need for long-term testing is more compelling. For ionised substances or surfactants the determination of a trigger value on the basis of other physico-chemical properties, e.g. Kd should be sufficient to ask for long-term tests. Taking all this into account, long-term toxicity tests should be asked for immediately for substances with log Kow > 3 (or BCF > 100) and a PEClocal or PECregional > $1/100^{th}$ of the water solubility.

The water solubility should, where possible, be based on the solubility in the aquatic toxicity test water rather than distilled water (presuming that this solubility is measured after filtration (0.45 μm) of the test solution or after centrifugation). When the logKow is not a good indicator of bioconcentration, or where there are other indications of a potential to bioconcentrate (see Section 3.8), a case-by-case assessment of the presumable long-term effects will be necessary.

6 TESTING STRATEGIES

6.1 INTRODUCTION

In this chapter testing strategies for PEC and PNEC are given that are in principle to be followed when the conclusion of the risk characterisation phase is that there is concern and there is a need to ask for further information to refine the risk assessment. As has been mentioned in the previous chapter a decision has to be made as to whether PEC, PNEC or both need to be revised. This decision by the competent authority must be transparent and justified and should be based on the principles of lowest cost and effort, highest gain of information and the avoidance of unnecessary testing of animals.

Separate from the testing strategies that need to be followed when risks are identified, the PBT assessment as described in Section 4.4 may identify the need for further information to clarify the potential PBT (Persistent, Bioaccumulative, Toxic) or vPvB (very Persistent, very Bioaccumulative) properties of a substance. When such testing is requested, and the substance turns out not to fulfil the PBT or vPvB criteria, the test results should be used in the subsequent PEC/PNEC calculations.

6.2 REFINEMENT OF PEC

In order to refine the PEC, in addition to comprehensive information on production and application, additional tests may lead to a better quantification of the elimination processes of a substance in the individual environmental compartments or in the sewage treatment plant. The exact degree of elimination may be determined by measurements in the influent and effluent of sewage treatment plants or by conducting appropriate tests on the degradation behaviour.

The testing strategy for biocides can be found in the Technical Notes for Guidance for Directive 98/8" (TNsG on Data Requirements, 2000, Chapter 3, Section 7.0.2, available on http://ecb.jrc.it/biocides/). This strategy could also be employed on substances, which potentially may meet the persistency criteria for PBTs. The kind of simulation test asked for should depend on the compartment of highest concern. If the sediment compartment turns out to be the compartment of highest concern, it could be decided to continue with a sediment simulation test depending on the physico-chemical properties of the substance as defined in the biocides testing strategy.

Furthermore it should be noted that a guidance document on how to assess and test relevant metabolites and transformation products is under preparation for plant protection products under Directive 91/414. This document could be modified later for use for biocides, and where appropriate for new and existing substances.

Guidance in relation to further degradation studies when refining the PEC for STP or one or more of the environmental compartments is given below. In general simulation tests should be considered based on the likelihood for such test data to actually refine the PEC(s) in a way that may influence the ultimate result of the risk assessment (see Section 2.3.1, sensitivity analysis).

Similarly, the experimental determination of the BCF can be requested in order to refine the PECoral for secondary poisoning (see Section 3.8).

Another possible option for the refinement of the PEC is the performance of simple monitoring (for example at point of release or in predicted worst-case environments). Long-term monitoring programmes should only be initiated:

- in the case of borderline risk assessments, where immediate risk reduction action cannot be justified;
- as a means of checking the effectiveness of risk reduction action;

taking into account monitoring programmes established under other EU legislation.

6.2.1 Aquatic compartment

In the following, a biodegradation testing strategy for the aquatic environment is presented in relation to standardised testing methods available (see also Sections 2.3.6 and 4.2.3).

However, it should also be considered at each stage whether further abiotic testing, e.g. direct or indirect aquatic photolysis or a, full adsorption/desorption test, could refine the PEC (local or regional). In that respect it has to be considered whether the photolytic or hydrolytic degradation products themselves may constitute a risk, and it should be considered to determine the ultimate degradation half-life of these degradation products.

Two cases can be distinguished:

PEC/PNEC > 1 and the substance is readily biodegradable

Further biotic testing is unlikely to affect the PEC, unless the producer/importer believes it is worth conducting a simulation test, which may generate a removal percentage greater than that assumed for readily biodegradable substances.

PEC/PNEC > 1 and the substance is not readily biodegradable

If the substance is inhibitory at a level below that used in the ready test, an STP simulation test that measures ultimate degradation should be performed at a non-inhibitory concentration. This will only help refine PEClocal if the concentration predicted in the sewage treatment plant is below the inhibition threshold.

Simulation tests for surface water and/or aquatic sediments may be needed to refine the PECs for surface water and/or sediment for the regional assessment. Internationally standardised methods have recently been developed and should be used for this purpose (see Section 2.3.6). The results from such testing can be used directly in the calculation of PEC for the system being simulated. Care will need to be taken, however, that the conditions of the test substance concentration reflect those likely to be found in the relevant compartment (STP, surface water, sediment and/or soil) so that the degradation half-life for full mineralisation can be established. For slowly degrading substances it is in general recommended that any metabolites/degradation products are identified and that their mineralisation half-lives are also established.

In deciding whether there is a need for further simulation degradation studies in one or more of the environmental compartments surface water (freshwater, marine water) and/or sediment it should be considered how a more precisely determined half-life for that compartment might influence the overall risk assessment of the substances. This should be done by taking into account the current production, use and environmental release and distribution of the substance.

Performance of an inherent test is generally not justified and consideration should be given to conduct a simulation test giving relevant information on the degradation kinetics.

A testing strategy on biodegradation of biocidal active substances has been developed, details of which can be found in the Technical Notes for Guidance on data requirements for Directive 98/88 on the placing of biocidal products on the market (TNsG on Data Requirements, 2000; http://ecb.jrc.it/biocides/).

6.2.2 Soil compartment

If the PEC/PNEC ratio for the soil compartment is greater than one, further degradation testing will refine the assessment in several ways:

- the estimation of the amount of substance entering the soil compartment via land-spreading of sludge can be refined by more sophisticated degradation or adsorption/desorption testing regarding sewage treatment plants;
- it can also be refined by investigating the potential for anaerobic degradation in the sludge, which is otherwise assumed to have no effect on the concentration of the substance. For testing of anaerobic biodegradation a standard test method is available (ISO 11734, 1995). This screening test method is designed to investigate the potential for anaerobic degradation in STP digesters, and may thus be relevant for a rough estimation of degradation in anaerobic STP sludge, which is deposed on agricultural soil. Tests for anaerobic degradation and inhibition of anaerobic STP bacteria could therefore possibly be considered on a case-by-case basis in the risk characterisation of certain substances.

A refined estimation of the fate of the substance once it has reached the soil compartment may also be possible using a simulation degradation test performed in soil (Draft EU Annex V C.23, OECD guideline 307, 2000b). Also in relation to the need for such a simulation test, it has to be considered how the results may influence *or* have an impact on the overall risk assessment of the substance. Also here account should be taken of the current production, use and environmental release and distribution of the substance.

A testing strategy on degradation of biocidal active substances has been developed, details of which can be found in the Technical Notes for Guidance on data requirements for Directive 98/88 on the placing of biocidal products on the market (TNsG on Data Requirements, 2000; http://ecb.jrc.it/biocides/).

- abiotic testing should also be considered. Tests include (direct) photolysis, and more refined adsorption/desorption in soil (see however the general remarks above).

6.2.3 Air compartment

For the air compartment experimental testing of direct photodegradation and chemical reactions originating in atmospheric photochemistry is complicated and should only be required if there is a serious indication of possible adverse effects related to the PEC in the atmosphere. Instead it is preferable to use QSARs where they are available.

6.3 REFINEMENT OF PNEC: STRATEGY FOR FURTHER TESTING

6.3.1 Introduction

A detailed strategy for further testing in order to refine the PNEC has been developed for the aquatic compartment. Guidance for deciding on further testing requirements although less specific than for the aquatic environment, is also provided for the sediment and terrestrial compartments and for secondary poisoning. Long-term tests are considered most applicable since a PNEC based on long-term ecotoxicity data is more reliable than a PNEC based on short-term data. The additional tests lead to lower assessment factors due to the lower uncertainty. These strategies are described in detail within the discussion on the effects assessment (Section 3) under the relevant compartment.

Refinement of the $PNEC_{water}$ for the aquatic compartment can be carried out by performing long-term tests with the most sensitive species or, if one or two NOEC(s) is/are already available, with a long-term test on species of trophic levels for which no NOEC was determined so far. The decision taking process can be supported by the use of (Q)SARs. The testing strategy is described in Section 6.3.2. The testing strategy proposed for the sediment compartment is described in Section 6.3.3.

The risk assessment concept for the terrestrial compartment includes also a strategy for deciding when to carry out short-term toxicity tests on terrestrial organisms. Short-term tests are not included in the base-set but should be conducted, if a potential risk to soil has been identified on the basis of a risk characterisation using the equilibrium partitioning method. Expert judgement is required to decide on the most appropriate long-term test(s) if it is considered necessary to refine the $PNEC_{soil}$ (see Section 6.3.4).

While any possible refinement of the PECoral/PNECoral ratio for secondary poisoning targets more the refinement of the PECoral rather than of the PNECoral, it may in some cases be more appropriate to refine the latter and conduct long-term or chronic toxicity tests. The decision on which test to conduct has to be taken on a case-by-case basis.

No internationally accepted standardised test guidelines and/or no adequate effects assessment methods are available at present for the air compartment. Consequently no testing strategy is proposed. If it is concluded that this compartment is at risk a decision will have to be taken on a case-by-case basis.

6.3.2 Aquatic compartment

6.3.2.1 Introduction

In the event that the $PEC_{water}/PNEC_{water}$ ratio is greater than one, either exposure data have to be refined or further testing specified. One or more additional tests may have to be performed in accordance with methods specified in Annex V to Directive 67/548 or in OECD guidelines (or equivalent test guidelines). The methods used must be appropriate to a refined risk assessment. Only those tests yielding results that may lead to a revision of the $PNEC_{water}$ should be performed. Under some circumstances it might be appropriate to consider a mesocosm or (semi) field test that assesses sensitive and ecosystem-specific endpoints that are different from those assessed in single-species tests.

Care must be taken, when attempting to revise the effects assessment by conducting additional aquatic toxicity testing, to ensure that species sensitivity is fully taken into account. Although the choice of tests is necessarily limited, it must reflect the anticipated exposure conditions and the chemical properties of the substance.

In determining whether additional testing is required, the following guidelines should be followed:

- additional testing should lead to a revision of the estimated $PNEC_{water}$ which, when based on long-term ecotoxicity data, is more reliable than the $PNEC_{water}$ when based on short-term data;
- the species with the lowest L(E)C50 in short-term studies should normally be examined first for the purposes of long-term testing. Differences in L(E)C50s can be determined by comparing their values: one value is considered to be significantly lower than another if it is more than ten times lower. However, these definitions can only provide a guide to the relative sensitivities of taxonomic groups. Expert judgement must therefore be used to determine whether they are sufficient in any given case;
- further testing would not normally be required on a species for which no short-term toxicity has been demonstrated (L(E)C50 > 100 mg/l). This may not apply to poorly water-soluble substances (water solubility < 1 mg/l) for which no short-term toxicity may have been demonstrated (see Section 5.6). In other cases, expert judgement should be used to determine whether further testing of a species is necessary.

For substances that have a potential to bioaccumulate, it should be recognised that long-term or delayed effects are possible. These effects might not have been apparent or predicted from the results of short-term studies or long-term tests appropriate for non-bioaccumulating substances. This is considered to be of particular importance when considering long-term fish and Daphnia toxicity since several sensitive stages of their development can be affected because of their high lipid content in the early stages of their life-cycles. Care needs to be taken, therefore, to ensure that the appropriate long-term test is selected and that steady state concentrations are achieved in the organisms for a period that is sufficient to allow the potential effects of bioaccumulation to be investigated. Normally a Fish Early Life Stage test (OECD 210, 1984g) would be considered appropriate for examining fish toxicity. However, the fish, juvenile growth test (EU Annex V C.14) (for substances with log Kow < 5) or egg and sac-fry stage test (EU Annex V C.15) (for substances with log Kow < 4) may also be considered.

The results from these long-term toxicity tests cannot exclude the possibility of delayed effects. When such effects are suspected, it may be appropriate to consider full life-cycle tests for fish according to the US EPA guidelines 670/4-73-001 (US EPA, 1973) or 600/9-78-010 (US EPA, 1978) and/or Daphnia (A guideline for a full life-cycle test for Daphnia is not available yet). Such testing would not be regarded as normal and should be necessary only in exceptional circumstances.

Not all endpoints (such as multi-generation effects or behavioural disturbances) are assessed using these tests and biomagnification processes can hardly be reproduced in laboratory scale experiments. Consequently, even with this information, delayed effects in the ecosystems cannot be ruled out.

6.3.2.2 Available long-term tests

The long-term tests available when seeking to refine the PNEC are limited. It is nevertheless important that the correct test is chosen to maximise the usable information and avoid unnecessary repeat testing.

Long-term fish testing

Fish early-life stage(FELS) toxicity test (OECD 210, 1992h)

A full life-cycle fish test is not currently available as standardised test method. In its absence the FELS toxicity test is considered as the most sensitive of the fish tests, covering several life stages of the fish from the newly fertilised egg, through hatch to early stages of growth. This is considered to cover most, but not all, of the sensitive points in the life-cycle and is also the only suitable test currently available for examining the potential toxic effects of bioaccumulation. It is, however, a long test, typically 60 days post-hatch for rainbow trout (Oncorhynchus mykiss), or approximately 30 days post-hatch for warm water fish, and is consequently the most expensive of those available. It should therefore only be requested where long-term fish toxicity data are required and the substance has the potential to bioaccumulate.

Fish, short-term toxicity test on embryo and sac-fry stages (EU Annex V C.15, OECD 212, 1998c)

This test measures the sensitive early life stages from the newly fertilised egg to the end of the sac-fry stage. It is considerably shorter, and hence less expensive, than the FELS toxicity test but is also considered less sensitive. The method offers an alternative to the FELS toxicity test for substances with log Kow less than 4.

Fish, juvenile growth test (EU Annex V C.14, OECD 215, 2000d)

This test measures the growth of juvenile fish over a fixed period, and is considered a sensitive indicator of toxicity. Although it is considered to be of insufficient duration to examine all the sensitive points in the fish life-cycle, it provides a shorter and less expensive option to the FELS test for substances of log Kow < 5.

Fish, prolonged toxicity test, 14-day study (OECD 204, 1984c)

This test cannot be considered a suitable long-term toxicity study since it does not examine a sensitive stage in the fish life-cycle. It is, in effect, a prolonged acute study with fish mortality as the major end-point examined. However, sub-lethal effects are monitored and the NOEC should be based on the absence of these effects. It should not be requested where a long-term fish study is required. It should only be requested where provision of further information on possible short-term effects is considered necessary.

Long-term Daphnia testing

Daphnia magna reproduction test (EU Annex V C.20, OECD 211, 1998b)

This test measures effects on juvenile production as well as parental immobility and mortality. It is frequently (and preferably) conducted over 21 days. Although it does not cover the full Daphnia life-cycle, it does cover the sensitive reproduction stage and is therefore considered a sensitive long-term study.

Algal testing

Algae toxicity test (EU Annex V C3, OECD 201, 1984a)

The algal growth inhibition test measures the inhibition of growth during the exponential phase under optimum standard conditions of light, temperature and nutrient concentrations. The test produces an EC50 that can be considered equivalent to a short-term L(E)C50. Often both ErC50 (estimated from specific growth rate) and EbC50 (estimated from biomass growth) are available, however the latter should not be used. The reason is that direct use of the biomass concentration without logarithmic transformation cannot be applied to an analysis of results from a system in exponential growth. Where only the EbC50 is reported, but primary data are available, a re-analysis of the data should therefore be carried out to determine the ErC50.

It is sometimes seen also when test was done according to standard test guidelines, that the exponential growth ceased in the control before the end of the test period. Likewise it may be seen that the validity criteria of the test were not fulfilled (pH increase etc.) or growth of the algae in the exposed concentrations was increased (due to e.g. loss of test substance from the test system) at the end of the test. In such cases only data from the part of the test where exponential growth and the validity criteria for the controls as well as for the exposed groups occurred should be used. In many such cases this may be achieved by excluding data from the last test day from the calculation of ErC50 and NOEC or ErC10. (Nyholm, 1985; Nyholm and Källqvist, 1989; Ratte, 1998; Weyers & Vollmer, 2000; Källquist; 1999, 2000; Weyers et al., 2000). If only EbC50 is reported and no primary data are available, it should be considered to perform a new algae study to obtain a valid ErC50 and NOEC or ErC10.

The algal growth inhibition test is not only a multi-generation test but also provides a measure of sub-lethal effect - reduction in population growth. It can therefore be considered a true chronic test, albeit of short duration. The NOEC may therefore be used in the assessment strategy, but with some modification compared to NOECs from long-term chronic tests with fish or Daphnia (i.e. availability of a NOEC for algae alone is not used as a justification deviating from using the lowest L(E)C50-value from short-term studies).

6.3.2.3 Decision table for further testing

The decisions to be made in respect of further testing requirements are detailed in **Table 34**. Although the basic criteria outlined above must always be taken into account, common sense must also be applied when considering individual situations. Decisions taken in respect of further testing will be different depending on species sensitivity. In all cases, the algal study from the base set is first considered as a short-term study and the EC50 used for calculation of the PNECwater. However, the algal study is technically a multi-generation test and thus, if there are other long-term NOEC data, the algal NOEC can be considered as a long-term NOEC in the revised assessment. Generally, this algal NOEC would not be used unsupported by other long-term data.

Chapter 4 (Use of (Q)SARs) gives full details on the use within the testing strategy of the QSAR estimates for substances with a non-specific mode of action and for estimating long-term fish and Daphnia toxicity.

Table 34 Decision table for aquatic toxicity testing when results from a full base-set (FBS [a)]) using an assessment factor on the lowest L(E)C50, show that PEC/PNEC>1

Variation in base-set data	Further testing	Data available for assessment	Assessment factor [b)]
No significant difference between the L(E)C50 values of fish, Daphnia or algae	Long-term fish test + long-term Daphnia test + determination of NOEC algae	FBS + algae + Daphnia + fish	10
Fish LC50 more than 10 times lower than L(E)C50 of Daphnia and algae	Long-term fish test + determination of NOEC algae	FBS + algae + fish	50
	If S/L [c)] ratio for fish > 20: long-term Daphnia test [d)]	FBS + algae + fish + Daphnia	10
Daphnia L(E)C50 more than 10 times lower than L(E)C50 of fish and algae	Long-term Daphnia test + determination of NOEC algae	FBS + algae +Daphnia	50
	If S/L [c)] ratio for Daphnia > 20: long-term fish test [d)]	FBS + algae + fish + Daphnia	10
Algae L(E)C50 more than 10 times lower than L(E)C50 of fish and Daphnia	Test on other algae species + long-term fish/Daphnia test [e)]	FBS + two algae [e)] + fish/Daphnia	10 [e)]
Fish LC50 more than 10 times higher than L(E)C50 of Daphnia and algae	Long-term Daphnia test + determi-nation of NOEC algae	FBS + algae + Daphnia	50
	If S/L [c)] ratio for Daphnia >20; long-term fish test [d)]	FBS + algae + fish + Daphnia	10
Daphnia L(E)C50 more than 10 times higher than L(E)C50 of fish and algae	Long-term fish test + determinati-on of NOEC algae	FBS + algae + fish	50
	If S/L [c)] ratio for fish >20: long-term Daphnia test [d)]	FBS + algae + fish + Daphnia	10
Algae L(E)C50 more than 10 times higher than L(E)C50 of fish and Daphnia	Long-term Daphnia test + long-term fish test + determination of NOEC algae	FBS + algae + fish + Daphnia	10

Notes to Table 34:

a) FBS = full base set which includes L(E)C50 values for fish, Daphnia and algae.

b) AF = the assessment factor must be applied to the lowest NOEC available at this stage, including the NOEC from the algae test.

c) S/L refers to the short-term to long-term ratio, i.e. the ratio between the L(E)C50 from a short-term test and the NOEC from a long-term test.

d) Generally testing of a third species will be unnecessary since the toxicity results from the first species should be protective. However, this cannot be a fixed rule given the toxicity variations within taxonomic groups as well as between them. Thus if a short-term L(E)C50: long-term NOEC ratio > 20 is found for the species tested, or from the algal study, then further testing of a third species might be necessary. The use of long-term fish or Daphnia QSARs could help in deciding which species need to be tested (see Chapter 4 "Use of QSARs"). It is considered that such a ratio may be indicative of an abnormal level of toxicity or a specific mode of action, and thus the acquisition of additional evidence is justified in order to improve the confidence in the calculated $PNEC_{water}$. Other factors such as the shape of the toxicity time curve and the presence of sub-lethal effects in the short-term toxicity study for the second species may also be considered. An assessment factor of 10 may be applied to the lowest of the three NOECs. Due consideration should be given to whether the resultant NOEC will lead to a further revision of the $PNEC_{water}$ before a toxicity study on a third species is requested.

e) This table is based on the presumption that an algal NOEC is available at the base-set. If this is not the case an assessment factor of 50 should be used.

6.3.3 Sediment compartment

If no long-term test with sediment organisms is available and the PEC/PNEC ratio established via the equilibrium partitioning method or from short-term tests shows concern for the sediment compartment, further testing is necessary. When selecting test species, the behaviour of the substance together with the feeding strategy of the test species should be considered. The following species are recommended:

- long-term test with *Lumbriculus variegatus* using spiked sediment;
- long-term test with *Chironomus riparius* or *Chironomus tentans* using spiked sediment;
- long-term test with a further benthic species using spiked sediment.

The selection of the test species should depend on the properties of the test substance.

The species mentioned represent different habitats and feeding strategies and are therefore exposed to sediment-bound substances by different exposure pathways. *Lumbriculus variegatus* is a true sediment feeder, while *Chironomus* sp. is a collector-gatherer that feeds mainly on material deposited on submerged substrate. The two species belong to different benthic taxa and the tests involve different life stages. Selection of the third test species should supplement the first two species in these aspects. Other test methods are quoted in Appendix VI.

In addition to the described tests with benthic invertebrates, consideration can be given to sediment tests with other benthic species that are important for the sediment compartment, e.g. microorganisms and plants. A prerequisite would be that the tests are true sediment tests and that all relevant exposure pathways are covered. Especially the tests with microorganisms must essentially cover endpoints / degradation processes relevant for the sediment compartment (e.g. respiration, nitrification, denitrification, nitrogen fixation, methane formation). In general, tests with microorganisms and plants should be used only as the third sediment test, i.e. to lower the assessment factor to 10. As standardized sediment tests for microorganisms and plants are not yet available, further research and development is needed in this field.

An alternative to the testing of a third species could be a test with a second sediment performed with the most sensitive of the species already tested, provided that the characteristics of the second sediment, which determine bioavailability for the substance in question (e.g. organic carbon content, composition, grain size, …), are very different from the first one.

Supplementary feeding of the organisms during the test should be avoided otherwise it may reduce the ingestion of contaminated sediment particles. Tests with species that need supplementary feeding should be designed in such a way that food taken up *via* the sediment by the test organisms is also spiked or contaminated with the test substance. To solve this problem e.g. an artificial sediment with pulverized leaves as carbon source as proposed by Oetken et al. (2000) could be used.

The composition of the sediment used for the tests should depend on the requirements of the test species and should therefore be gathered as described in the respective test methods. The use of artificial sediment is recommended. However, if there is experience with a special natural sediment, this can also be used for the test. Then the properties of this sediment have to be described in detail.

The organic carbon content of the sediment may influence the bioavailability and therefore the toxicity of the test substance. Therefore, for comparison of sediment tests, the organic carbon content of the test sediment should be within a certain range. The draft OECD guideline 218 (2001e) for the test with *Chironomus* using spiked sediment recommends an organic carbon content of the test sediment of 2 % (+/- 0.5 %). In **Table 5** the organic carbon content of a standard sediment is set to 5 %. It is recommended that the organic carbon content of the test sediments is between these two values.

Various techniques can be used to spike sediments, e.g. wet spiking and dry spiking. A flexible approach should be adopted due to variations in physico-chemical properties of test substances. However, it has to be guaranteed that the substance will not desorb from the sediment particles

during the test as this would lead to an underestimation of the toxicity. To limit such desorption an adequate equilibration period before the start of the test is recommended. In addition the actual concentration of the test substance in the sediment should be monitored at least at the beginning and at the end of the test to check the efficiency of the contamination technique and the stability of the test substance concentration.

6.3.4 Soil compartment

At an initial stage and in respect to the current proceedings in the aquatic compartment, a minimum data set for risk assessment for soil organisms could be based on short-term toxic effects data. $PEC_{soil}/PNEC_{soil}$ ratios are derived from either ecotoxicological data or the equilibrium partitioning method (see Section 3.6.2.).

Two cases can be identified where it might be considered necessary to revise the $PNEC_{soil}$,:

(1) short-term tests on primary producers, consumers and decomposers should be performed if the equilibrium partitioning method is applied because of the absence of toxicity data for soil organisms and the $PEC_{soil}/PNEC_{soil}$ is > 1. In some cases long-term tests might be preferred immediately when, for example, soil organisms or part of the life-cycle of a plant or microbial processes are suspected to be particularly sensitive to the test compound. This is especially true, if the substance in question exhibits a log Kow greater than 5 (equivalent to a log Koc > 4) or exhibits a corresponding binding behaviour;

(2) further testing may be necessary if the $PNEC_{soil}$ is based on toxicity data for soil organisms using assessment factors and the $PEC/PNEC_{soil}$ > 1. Long-term tests should be considered in particular if the available $PNEC_{soil}$ is based on short-term effects. Depending on the effect that a substance has on vascular plants, earthworms or processes mediated by microorganisms, the information about the effect on the most sensitive organisms has to be improved by conducting appropriate tests for the respective endpoints. The choice of the test species will be made on a case-by-case basis taking into account the availability of a suitable test method, the sensitivity of aquatic and/or sediment living organisms that may be predictable for the sensitivity of equivalent groups of soil organisms, the indicative nature of the assessment factors and the uncertainty in the proposed approach.

Internationally accepted methods (OECD and ISO) should preferably be used but results from other methods that are in the process of being standardised might also be appropriate. Several research programmes have been initiated that are aimed at the development of soil tests: the Netherlands Integrated Soil Research Programme (NISRP; Eijsackers, 1989) and the Swedish Mark Test System (MATS; Rundgren et al., 1989). More recently, ten European laboratories have formed a network (SECOFASE, Løkke and van Gestel, 1993) funded by the European Union to develop, improve and standardize tests systems for assessing sublethal effects of chemicals on fauna in soil ecosystems. As a result of this European research project, test protocols, indications on species sensitivities, reproducibility of the tests and also advice for the choice of test species has been published in the “Handbook of soil invertebrate toxicity tests” (Løkke and van Gestel, 1998).

Microbial assays

Microbial processes are considered as short-term tests. A NOEC from these tests could be considered as long-term results for microbial populations.

Protozoans live mainly in the soil pore water and results from ciliate growth inhibition tests are relevant for the risk assessment for STPs (see Section 3.4.). Ecotoxicity tests with/on Protozoans will not be used for the risk assessment in the soil compartment unless specific assay have been developed for soil Protozoans.

Determination of nitrogen mineralization and nitrification in soils and the influence of chemicals on these processes (draft EU Annex V C.21; OECD 216, 2000e; ISO 14238, 1997)

Microorganisms use the soil organic matter to satisfy their own energy and nutrient requirements. Organic N is then mineralised to ammonia and oxidised to nitrate. The test is designed to determine the influence of a substance on the mineralization rate of a soil with a low organic carbon content that is representative of a worst case for the bioavailability of the substance. Nitrate concentration is measured in soils treated with the test substance after a 28 days incubation period. The result is compared to the nitrate concentration in a control and the degree of inhibition is calculated.

Determination of carbon transformation activity (draft EU Annex V C.22; OECD 217, 2000f; ISO 14239, 1997)

Under aerobic conditions ultimate degradation of organic matter by decomposer organisms leads to carbon dioxide formation. Respiration measurement is used to assess the activity of microbial populations. Carbon dioxide or oxygen uptake can be measured on soils that are incubated under controlled environmental conditions. Inhibition of mineralization is then determined.

Determination of potential nitrification, a rapid test by ammonium oxidation (ISO/CD 5685, 2000)

Ammonium oxidation is the first step in autotrophic nitrification in soil. The method is based on measurement of the potential activity of the nitrifying population as assessed by the accumulation of nitrite over a short incubation period. The method does not assess growth of the nitrifying population. Inhibitory doses are calculated.

Determination of abundance and activity of the soil micro-flora using respiration curves (ISO/CD 17155, 2000)

This method is used to assess the effect of chemicals on the soil microbial activity by measuring the respiration rate (CO_2 production or O_2 consumption). The chemicals may kill the micro-flora, reduce their activity, enhance their vitality or have no effect (either because the toxicity of the substances is low or some species are replaced by more resistant ones). EC10 and EC50 are determined when toxicity is observed.

Invertebrate assays

Ecotoxicity tests (but not necessarily standardised tests) exist for Nematodes, Annelids, Molluscs and Arthropods. Other invertebrate tests based on, for example, Annelids, Arthropods or other phyla could equally be used. Standardised tests that are currently available are described below.

Earthworm acute toxicity test (EU Annex V C.8; OECD 207, 1984d; ISO 11268-1, December 1993)

The test is designed to assess the effect of chemicals on the survival of the earthworms *Eisenia* spp. Adult worms are exposed to a range of concentrations of the test substance mixed into the soil. Mortality and effects on biomass are determined after 2 weeks exposure. Where possible, LC50 and EC50 values are determined. *Eisenia* spp. is considered to be representative of soil fauna and earthworm species. The organism was however selected more for pragmatic reasons (easily cultured in laboratory conditions) than for its sensitivity or it being representative of soil dwelling organisms.

Insect larvae acute toxicity test (NF X 31-260 accepted as a new work item ISO/TC/90/SC4/WG2)

Oxythyrea funesta is widely distributed in Europe. With a phytophage feeding habit, this organism plays an important role in determining the physical characteristics of soils (structure, texture, aeration,…). Survival of insect larvae (*Oxythyrea funesta*) exposed to contaminated soils is assessed in a test lasting 10 days. A LC50 is then determined by comparing survival in treated soils with that of the control.

Earthworm reproduction test (ISO 11268-2, July 1998, draft OECD, 2000i)

The effect of chemicals on the reproduction of adult compost worms (*Eisenia fetida* or *E. andrei*) is assessed over a period of 8 weeks. Adult worms are exposed to a range of concentrations of the test substance mixed into the compost. Mortality and growth effects are determined after 4 weeks exposure. The adults are then removed and the number of offspring determined following a further 4 weeks exposure period. The NOEC is determined by comparing the reproductive output of the worms exposed to the test substance to that of the control.

Inhibition of reproduction of Collembola (Folsomia candida) (ISO 11267, 1999)

Collembola is an important group of arthropods in temperate soils. Several species have been used in toxicity experiments including *Folsomia candida* for which a standard reproduction test has been developed. A treated artificial soil is used as the exposure medium and a NOEC is determined.

Enchytraeidae reproduction test (draft OECD 220, 2000h), ISO/CD 16387, 2001)

Enchytraeids are soil dwelling organisms that colonise a wide range of soils. They are easy to handle and breed in laboratory conditions and their generation time is shorter than that of the earthworms. The effect of chemicals on the reproduction of adult enchytraeid worms is assessed over a period of 6 weeks. The principle of the test is the same as for the earthworm reproduction test: adult worms are exposed to a range of concentrations of the test substance mixed into the soil. Mortality and morphological changes are determined after 3 weeks exposure. The adults are then removed and the number of offspring, hatched from the cocoons in the soil is counted after an additional 3 weeks exposure. The NOEC is determined by comparing the reproductive output of the worms exposed to the test substance to that of the control.

Effects of pollutants on juvenile land snails (Helix aspersa) (NF X 31255/1, Draft April 2001)

Inhibition of growth of the snails is observed through food contamination (1) or soil contamination (2). The French standard protocol will be proposed within ISO as a new work item.

A soil bioassay for the nematode species *Caenorhabditis elegans* has been developed with mortality or sublethal endpoints (Løkke and Van Gestel, 1993).

Plant assays

Inhibition of root growth of higher plants (ISO 11269-1, November 1993)

Pre-germinated seeds are planted in control or contaminated soils in laboratory conditions. Growth rates of the roots are determined after an appropriate incubation period (depending on the species: 5 days for *Hordeum*). Results obtained in contaminated soils are compared to that of the control to determine IC50 or NOEC parameters.

Inhibition of emergence and growth of higher plants (ISO 11269-2, December 1995, draft OECD 208 A and B, 2000i)

Inhibition of seedling emergence and early growth of higher plants is determined by comparing seedling emergence, biomass and visual detrimental effects on seeds placed on treated soils with seeds placed on control soil. Exposure through soil that has been previously spiked is the general rule. However, foliar application might be more relevant in some cases, depending on the main uses of the substance. In these cases, the effects on plants following deposition of test substance on the leaves and above ground portions of plants could be assessed using other standardised protocols. For example, inhibition of vegetative vigour of higher plants can be determined by comparing biomass and visual detrimental effects in controls plants with those in plants that had been sprayed with the test substance (OECD 208B).

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Appendix I Emission factors for different use categories

This appendix consists of:

- release tables (A and B),
- a list of synonyms for functions of substances to obtain the best entry to the A- and B-tables (Appendix I-a and Appendix I-b),
- a scheme for use of all relevant emission data for a substance (Appendix I-c).

1. Introduction to the release tables

For all industrial categories distinguished in Chapter 5 estimates have been generated for:

1. the emission factors for the following stages of the life-cycle, i.e. (1) production, (2) formulation, (3) industrial use, (4) private use, service life and (5) waste treatment; these estimates have been collected in the "A-tables". When possible defaults occurring in emission scenario documents of the TGD have been implemented.
2. the fraction of the main source and the number of emission days (point sources); these estimates have been collected in the "B-tables". When possible data on the model source of emission scenario documents of the TGD have been implemented.

Many tables are applied for more than one category, but are given only once (at the first occurrence). For other categories, reference is made to the number of those tables.

Within one industrial category (IC) many different processes may take place involving many substances with very variable functions. Thus, the emission factors also may be very variable depending on process and process conditions. Function and physico-chemical properties may have a considerable influence. Further information on the Main Categories is given in Section 9. Section 10 includes further guidance for the determination of the correct Industry Category - Use Category combination. Background information on the A- and B-tables is provided in Section 11.

It should be noted that only for a limited number of industrial categories and specific applications (use categories) studies have been performed (resulting in so-called emission scenario documents (ESDs or use category documents). These emission scenario documents are presented in Chapter 7. They provide a solid basis for the estimates. Emission scenario documents give a good description of processes and the function of substances involved.

2. Types of substances and levels of production and use

New substances are usually produced at a rather low level. For existing substances high production volume chemicals (HPVC) have also to be considered. At present the IUCLID database contains over 2,500 existing substances that are produced or imported at amounts in excess of 1,000 tonnes/year. For the B-tables, default values for every industrial category have been introduced, above which a substance is considered to be an HPVC (unless the substance is considered as a HPVC by the notifier or when a tonnage is indicated for a HPVC in the relevant emission scenario document of the TGD). In Appendix I-c this is presented in 1: Characterisation. If the (production) volume of a substance is rather high (HPVC), it may be unrealistic to use the standard size for the STP. A correction may be made in a more refined stage of the assessment.

In the text the term "volume" will be used instead of "production volume", as the volume applied in the EU is considered. This means that the volume equals the production volume + the

volume imported in the EU - the volume exported from the EU (the substance as such, not the quantities imported in products). This is presented in Appendix I-c in 2: Tonnage.

A substance can have applications in more than one industrial category (IC) and/or use category (UC). As an assessment has to be made for all relevant applications of the substance, the input of fractions for different industrial and use category combinations must be realised according to 3: Use and stages of the life-cycle in Appendix I-c.

3. Aspects of production

If specific data on emissions at production are known, these can be used instead of the tables (see Appendix I-c under 4: Production characteristics at "Specific emission information"). Also for the fraction of the main source specific data may be entered, either as the capacity (tonnes/day) or as the period (days/year) in which the substance is produced (see Appendix I-c under 4: Production characteristics at "Production capacity").

4. Aspects of formulation

For this stage of the life-cycle specific data may be entered on the fraction of the main source and the emissions/emission factors, see Appendix I-c under 5: Formulation characteristics. For the emissions, a refinement may be achieved by discriminating between cleaning with/without water and soap. This has not been done yet.

In case a substance is applied in a formulation at a rather low level, unrealistic values for the fraction of the main source and the number of days will be derived from the tables using the tonnage as such. Therefore a correction should be made; a suggestion is to correct the tonnage as input for the B-table in the following way. For example if the percentage of substance in the formulation is 0.1, the volume (tonnes/year) is multiplied by 100/0.1. This tonnage may then be used to estimate the fraction of the main source and the number of days using the tables. It is possible to calculate an average in the case where a range of contents has been specified. This has been worked out in Appendix I-c in 5: Formulation characteristics at "Content in formulated product".

5. Aspects of industrial use

Industrial/professional use is referred to as "processing" in the A- and B-tables. Specific data on the fraction of the main source and the emissions may be used as input (see Appendix I-c in 6: Processing characteristics). This will be repeated for every specified IC-UC combination. In case a specific scenario for an IC-UC combination exists, specific data will be asked.

6. Aspects of service life

The life cycle stage service life is only considered for articles produced in textile industry.

7. Aspects of private use

Specific data on the fraction of the main source and the emissions may be used (see Appendix I-c in 6: Private use characteristics). This will be possible for every specified IC-UC combination for which the stage of private use is relevant.

8. Aspects of waste treatment

Specific data on the fraction of the main source and the emissions may be used (see Appendix I-c in 6: Recovery characteristics). This will be possible for every specified IC-UC combination for which the stage of waste treatment is relevant. For waste treatment only situations where a material – which contains the chemical of interest – is recovered and processes to make it suitable for re-use in its original application (recycling) or another application are taken into account.

9. Interpretation and use of the classification in "Main categories"

The main categories (MCs) were intended originally to provide a general impression of the relevance of the exposure during the whole life-cycle. The categorisation procedure outlined in Chapter 5 allows for one entry of the Main category (MC) only, for all stages of the life-cycle.

In the context of environmental risk assessment Main Categories are often used to characterise release scenarios for the estimation of emissions to the environment at individual stages of the life-cycle, i.e. at production, formulation and use. They can therefore be allocated to release fractions, which are used as default values where specific information is lacking.

MC I "Use in closed systems"

This MC refers to the stage of production and industrial/professional use. At the stage of production a substance should be assigned only to this category if it remains within a reactor or is transferred from vessel to vessel through closed pipework. The HEDSET distinguishes between three subcategories for intermediates.

For the stage of industrial/professional use this MC refers to substances that are used in closed systems, e.g. the application of a substance in a transformer or the circulation circuit of refrigerators.

MC II "Use resulting in inclusion into or onto a matrix"

Use consisting of inclusion into or onto matrices means all processes where chemicals are incorporated into products or articles from which they (normally) will not be released into the environment. This is applicable to the stage of formulation, e.g., when a substance is included in the emulsion layer of a photographic film. It also may refer to the stage of processing, e.g., when a paint additive ends up in the finished coating layer.

MC III "Non-dispersive use"

Non-dispersive use refers to chemicals which are used in such a way that only certain groups of workers, with knowledge of the process, come into contact with these chemicals. This means that the use of these chemicals is related to the number (and size) of the emission sources. So, this MC indicates industrial use at a limited number of sites (where emission reduction measures may be common practice).

MC IV "Wide dispersive use"

The term wide dispersive use should be used for a wide range of activities particularly when end users come into contact with the products. This means a large number of small point sources like households or line sources like traffic.

Although the HEDSET allows for one entry of the MC only for all stages of the life-cycle, the approach of MCs is used in EUSES in many cases for several stages of the life-cycle. As can be seen from Table 1 interpretation is often different.

Table 1 Interpretation of main category (MC) for relevant stages of the life-cycle

MC	Life-cycle stage	Interpretation
Ia	Production	Non-isolated intermediates (Industrial category 3 or 9 & Use category 33)
Ib	Production	Isolated intermediates stored on-site, or substances other than intermediates produced in a continuous production process
Ib	Formulation	Dedicated equipment and (very) little cleaning operations
Ic	Production	Isolated intermediates stored off-site, or substances other than intermediates produced in dedicated equipment
Ic	Formulation	Dedicated equipment and frequent cleaning operations
II	Formulation	Inclusion into or onto a matrix
II	Processing [1)]	Non-dispersive use (industrial point sources), or processing of intermediates in multi-purpose equipment
III	Production	Multi-purpose equipment
III	Formulation	Multi-purpose equipment
III	Processing [1)]	Non-dispersive use (industrial point sources), or processing of intermediates in multi-purpose equipment
IV	Processing [1)]	Wide dispersive use (many small point sources or diffuse releases; normally no emission reduction measures)

1) Processing refers to industrial / professional use

10. Remarks on the industrial categories

This paragraph defines the scope of the Industry Categories (ICs) and presents some short remarks on the ICs in relation to the A- and B-tables. The definition is based on the examples specified in the HEDSET for substances classified in the appropriate ICs.

One of the main problems using the A- and B-tables is the fact that it is often difficult to determine the correct tables to be used, i.e. to determine the correct IC-UC combination (industrial category-use category). The cause can be divided in two:

1. Correct categorisation is impossible because no suitable use category can be determined on account of the notification. Furthermore, problems may arise when the application of a substance takes place in a process that occurs in more than one industrial category.

2. The specification of the industrial category and/or use category by the notifier is wrong, and determination of the proper combination fails due to the fact that the detailed information of the notification may be cryptic.

A table is presented for every IC in which for every possible stage of the life-cycle the MCs are marked (with 'X'), which can be chosen or which are used automatically by the program on account of the choice made for the UC. If an MC can not be chosen or if no MC is needed a dot (.) has been placed in the table. Processing refers to industrial / professional use.

IC 1. Agricultural industry

Agricultural industry deals with the activities of growing crops (vegetables, grains, etc.) and raising cattle (for dairy products, meat and wool). It also comprises all allied activities such as pest control (application of pesticides, veterinary medicines), manuring, etc.

There are no emission scenarios and use category documents for this IC. Emissions due to the application (stage of processing) of pesticides are beyond the scope of the TGD. Several UCs are distinguished in the release scenario of the A-tables, e.g. UC = 19 Fertilisers and UC = 41 Pharmaceuticals.

Table for IC 1 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	**Main category**					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.

IC 2. Chemical industry: basic chemicals

The HEDSET considers two different ICs for chemical industry, the industry where substances are produced through chemical reactions. The raw materials for chemical industry come from petrochemical industry (IC 9 "Mineral oil and fuel industry"), from plant or animal materials, or coal. IC 2 is dedicated to *basic chemicals*, where the definition for use of the release estimation tables is based on the examples given in the HEDSET: basic chemicals are substances used generally throughout all branches of chemical industry and usually in considerable amounts. Important basic chemicals are solvents (UC 48) and pH-regulating agents (UC 40) (acids, alkalis).

There are no emission scenario and use category documents for this IC. In case a basic chemical is formulated A- and B-tables have been provided. Recovery is not considered as a feasible emission stage; emissions of chemicals such as catalysts are included in the emissions at the stage of processing. No distinction between UCs has been made in the emission tables so far; however, apart from UC = 48 "Solvents" most chemicals will have to be classified as UC = 40 "pH-regulating agents", UC = 55/0 "Others", and probably as UC = 43 "Process regulators".

Table for IC 2 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.

IC 3. Chemical industry: chemicals used in synthesis

The definition for *chemicals used in synthesis* based on the examples given in the HEDSET is: chemicals used in synthesis are substances either regulating the chemical reaction process (e.g. catalysts) or being used as an intermediate (i.e. chemicals that are formed and can be isolated at an intermediate step between starting material and the final product in a sequence of chemical processes). The HEDSET includes monomers in intermediates, which is only valid in the release estimation tables for the stage of production. For the processing stage the tables of IC 11 "Polymers industry" are used (see also subparagraph 4.2.5).

Apart from UC = 33 "Intermediates" most chemicals in this IC will have to be classified as UC = 43 "Process regulators" or UC = 55/0 "Others". Formulation may be applicable for some chemicals, whilst recovery is unlikely.

Table for IC 3 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 33)	.	X	X	.	X	.
Production (UC = 33)	X	X	X	.	.	.
Formulation (UC ≠ 33)	.	X	X	.	X	.
Processing	.	X	X	.	X	.

IC 4. Electrical/electronic industry

In electrical/electronic industry a wide range of products is manufactured. It comprises both the manufacture of components like resistors, transistors, capacitors, diodes, lamps, etc. and the production of televisions, radios, computers (PC's as well as mainframes), radar installations, complete telephone exchanges, etc. In the manufacturing processes constituent processes may take place. The main constituent processes are electroplating, polymer processing, and paint application. The emissions of substances used in these separate processes are ***not*** covered in IC 4, but in the following ICs:

- IC 8. "Metal extraction, refining and processing industry": electroplating and other metal processing (e.g. use of metalworking fluids);
- IC 11. "Polymers industry": polymer processing (shaping of thermoplastics and curing of prepolymers e.g. for the embedding of electronic components);
- IC 14. "Paints, lacquers and varnishes industry": application of coating products by all means of methods like spraying, curtain coating, etc.

There are no emission scenario and use category documents for IC 4. There are many different applications, however, in this IC, which may be characteristic and specific for it, e.g., the

production of printed circuit boards, semiconductors and the application of dielectric fluids in transformers and capacitors.

Table for IC 4 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	.

IC 5. Personal/domestic

In this IC the use and application of substances in household for maintenance and care of houses, furniture, kitchenware, gardens, etc., and personal care (hygiene, make-up, etc.) is covered. In many cases chemicals used in this IC will be present in formulations, e.g. in cleaners (soaps, detergents, washing powders, etc.), cosmetics, and products for the care of leather, textile and cars. Emissions will be very diffuse and only for wastewater the emissions to an STP are regarded as a point source. The release scenario in the A-tables considers 18 specific UCs. It is assumed that emissions take place during the whole year.

The application of substances for some specific purposes is covered in the following ICs at the stage of private use:

- IC 9. “Mineral oil and fuel industry”: fuels and fuel additives;
- IC 10. “Photographic industry”: photochemicals;
- IC 14. “Paints, lacquers and varnishes industry”: paint products.

Table for IC 5 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Private use	.	.	.	.	.	.

IC 6. Public domain

This IC covers application and use of substances in a variety of places by skilled workers, such as offices, public buildings, waiting rooms, various workshops such as garages, professional cleaning and maintenance of buildings, streets, parks, etc.

Most chemicals in this IC will be present in formulations, e.g. in “cleaners” (UC = 9 “Cleaning and washing agents and disinfectants”), non-agricultural biocides (UC = 39 “Biocides, non-agricultural”), and products for the maintenance of roads, buildings, etc. Different numbers of emission days are used for the identified UCs. The emissions in this IC will still be diffuse, but

the number of days over which emissions occur are expected to be different for the UCs (many products will be used only during working days or even during a short time period). UCs 9 and 39 have been distinguished besides UC = 55/0 "Others" in the release scenarios in the A- and B-tables.

Table for IC 6 of the MCs for the possible stages of the life-cycle which may be chosen on account of the chosen UC (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.

IC 7. Leather processing industry

The leather processing industry is considered to be the industry where leather is made out of raw hides, leather is dyed and where products are made out of leather (e.g. shoe manufacture).

For this IC an emission scenario document exists (focusing on leather dyeing, UC 10 "Colouring agents"). A general scenario is presented in the A- and B-tables with default values for common functions of chemicals like tanning (UC = 51 "Tanning agents". The release scenarios of the A- and B-tables make no distinction between UCs, only between MC = 2 and 3. Leather care such as for shoes belongs to IC = 5 "Personal/domestic".

Table for IC 7 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 10)	.	X	X	.	X	.
Production (UC = 10)	.	.	.	.	.	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	.

IC 8. Metal extraction, refining and processing industry

This IC covers the extraction of metals from ores, the manufacture of primary/secondary steel and non-ferro metals (as well "pure" metals as alloys), and the manifold of metal working processes ("shaping") like cutting, drilling, rolling, etc.

There are emission scenario and use category documents for one aspect of the processes in this IC, namely the application of metalworking fluids. The first is only for water based fluids and the local situation. On the basis of the use category document the release scenarios in the A- and B-tables distinguish the main function of (substances used in) metalworking fluids as being cooling and lubrication: UC = 29 "Heat transferring agents" and UC = 35 "Lubricants and additives".

Table for IC 8 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation (UC ≠ 29 & 35)	.	X	X	.	X	.
Formulation (UC = 29 / 35)	.	.	.	.	.	.
Processing	.	.	.	X	X	.

IC 9. Mineral oil and fuel industry

Mineral oil and fuel industry involves the petrochemical industry, which processes crude mineral oil. By means of physical and chemical processes (e.g. separation by means of distillation, cracking and platforming) a wide range of hydrocarbons serving as raw materials for the chemical industry and (often after adding a series of additives) fuels for heating and combustion engines, are produced.

There are no emission or use category documents for this IC. General release scenario tables are used in the A- and B-tables and do not make a distinction between UC = 27 “Fuels”, UC = 28 “Fuel additives” and UC == 35 “Lubricants and additives” or any other UCs.

Table for IC 9 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	**Main category**					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.
Private use	.	.	.	.	.	.

IC 10. Photographic industry

The photographic industry is the industry where photographic materials are manufactured (“solid” materials like films and photographic “papers”, but also preparations - either in a solid or a liquid form - for film and paper processing baths. The processing of films and photographic paper is also assigned to the photographic industry, including professional processing in so-called printshops. The treatment of films and photographic paper by the public at large is considered at the stage of private use.

There are both emission scenario and use category documents for this IC. As the first scenario only covers wastewater and the local situation specific release scenarios are found in the release scenarios of the A- and B-tables. The only specific UC in the scenarios is UC = 42 “Photo-chemicals”.

Table for IC 10 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation (“aqueous solutions”)	.	X	X	.	X	.
Formulation (“solid materials”)	.	.	.	.	.	.
Processing	.	.	.	X	X	.
Private use	.	.	.	.	.	.

IC 11. Polymers industry

In this report and in EUSES the polymers industry comprises the branch of chemical industry where ‘plastics’ (thermoplastics) are chemically produced, and industries where processing of thermoplastics and prepolymers takes place by means of a wide range of techniques (see below). These processes are all dealt with in IC 11 and not in branches of industry where polymers are produced (chemical industry) or processed (IC 4, 16 and 0).

On the basis of the available use category document and expert judgement general release scenarios have been provided in the A- and B-tables. First, there are tables for polymerisation processes, i.e. the processing stage of substances, which are converted into polymers by polymerisation reactions, polyadditions, polycondensations, etc. This has been done in order to be able to treat them specifically apart from substances produced in ‘chemical industry’ (in principle they may be regarded as process intermediates). Several types of functions, UCs and two polymerisation processes are distinguished.

Second, there are tables for the processing of polymers, i.e. “shaping” by all kinds of processes such as e.g. injection moulding, blowing, and extrusion. Although processing of polymers may occur in several ICs, e.g. IC 4 ‘Electrical/electronic industry’ and IC 16 ‘Engineering industries: civil and mechanical’, only one release scenario was introduced at the present IC. Several types of functions, UCs and thermoplastics and thermosetting resins are distinguished in the scenario.

Table for IC 11 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing (“polymerisation”)	.	.	.	.	.	.
Processing	.	.	.	.	.	.
Recovery	Not yet considered					

IC 12. Pulp, paper and board industry

Strictly speaking only the production of pulp, paper and cardboard out of wood or waste paper belongs to this IC. As the HEDSET categorisation does not specifically distinguish the reprographic industry this important activity has been separated from the general category 0 “Others”.

For this IC both emission scenario and use category documents are available. The emission scenario document deals with wastewater and the local situation. The release scenarios in the A- and B-tables are applicable to the stage of processing printing and allied processes, and the production of pulp, paper and board (including paper dyeing). The stage of recovery (paper recycling) is also considered in the tables.

Two UCs are specifically considered, i.e. UC 10 "Colouring agents" used as pigments in inks and as dyes for paper mass colouring, UC 20 and 31 ("Fillers" and "Impregnation agents") both used in paper production and UC 45 "Reprographic agents" which is a "collection" of all kinds of uses and functions of substances in printing and allied processes.

Table for IC 12 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	**Main category**					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 10)	.	X	X	.	X	.
Production (UC = 10)	.	.	.	.	.	.
Formulation	.	X	X	.	X	.
Recovery	.	.	.	.	.	.

IC 13. Textile processing industry

This IC covers treatment of fibres ("cleaning", spinning, dyeing, etc.), weaving, and finishing (e.g. impregnation, coating, etc.).

For this IC both emission scenario and use category documents are available. The release scenarios in the A- and B-tables are specific for IC 10 "Colouring agents" and general for other relevant UCs.

Table for IC 13 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	**Main category**					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 10)	.	X	X	.	X	.
Production (UC = 10)	.	.	.	.	.	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.
Private use (only UC = 10)	.	.	.	.	.	.

IC 14. Paints, lacquers and varnishes industry

Apart from the manufacture of coating products (stage of formulation) such as paints this report and EUSES also consider application of these products as belonging to this IC. This has been done because otherwise many release scenarios would have to be introduced in many other ICs. These could include for example IC 5 "Personal/domestic" for private use, IC 6 "Public domain" for professional application by house painters and in (small) workshops, and many industrial applications. The latter could include IC 16 "Engineering industries: civil and mechanical" in the

manufacturing of motor cars, constructions, etc. and IC 8 “Metal extraction, refining and processing industry”.

There is an emission scenario on paint manufacture and application (stages of formulation and processing respectively) and a use category document for paint manufacture. The A- and B-tables have release scenarios for both water-based and solvent-based coatings systems and distinguish 8 specific UCs; both industrial use (stage of processing) and private use. The stage of formulation concerns the manufacture of the coating products.

Table for IC 14 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	**Main category**					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.
Private use	.	.	.	.	.	.

IC 15. Engineering industries: civil and mechanical

Industrial activities belonging to this IC include wood processing industries (e.g. wooden furniture), motor car manufacture, building industry, etc. There are no emission or use category documents for this IC. Processes such as coating application take place in many of these activities; these processes are dealt with in the IC where the specific process belongs (coating application: IC 14 “Paints, lacquers and varnishes industry”). For the present IC the same general release scenarios as for IC 15 “Others” are used in the A- and B-tables.

Table for IC 15 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	**Main category**					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	X

IC 16. Others

All processes and activities, which can not be placed in one of the previous ICs, belong to this IC. An example is the food processing industry. General release scenarios are used in the A- and B-tables.

Table for IC 16 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 1):

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	X

11. Relationship between industrial categories

In practice all chemicals originate from IC 2 & 3 "Chemical industry" and go from there to one of the other ICs (or remain in chemical industry). Substances such as monomers, cross-linking agents, and curing agents take a special position. These substances are basic chemicals (raw materials) for IC 11 "Polymers industry" for the production of *polymers* by polymerisation reactions and other reactions like polyaddition and polycondensation. Despite the fact that this may be seen as the stage of production in IC 3 (UC 33 "Intermediates") they have been introduced in the emission tables of IC 11 "Polymers industry" as UC 43 "Process regulators". Besides the production of polymers this IC also deals with the processing of the polymers (thermoplastics) and prepolymers (prepolymers are macromolecular substances such as polyester and epoxy resins which are transformed in thermosetting resins with the aid of curing agents, such as initiators - mainly organic peroxides - and cross-linking agents - mainly the monomer styrene - for polyesters, and curing agents like amines for epoxy resins). The processing stage of (pre) polymers involves the manufacture of all kind of articles and parts of objects from the basic materials.

The releases in both IC 5 "Personal/domestic" and IC 6 "Public domain" have a diffuse character. In IC 5 the use of chemicals in households is covered and in IC 6 the use in offices, public buildings, parks, railway stations, in the street, etc. The main differences will be found in the amounts (e.g. because of the size of the building) and the number of days that emissions occur.

12. History of the A- and B-tables

In the development of the quantitative risk assessment system for new substances DRANC (Dutch Risk Assessment System for New Chemicals) (Toet et al., 1991; Vermeire et al., 1992) emission tables were developed for a limited number of applications. The applications considered were textile dyes, photo-chemicals, metalworking fluids, hydraulic fluids, paper-chemicals, and intermediates. For these applications so-called use category documents were available. Nearly at the same time PRISEC (PRIority Setting system for Existing Chemicals) was developed (Van de Meent and Toet, 1992). For this system emission tables were developed for the 15 industrial categories distinguished at that time in the HEDSET (EC/OECD Harmonised Electronic Data Set). The emission factors were established by means of expert judgement and tended to the worst-case situation. For the local release estimation tables were supplied containing expert judgement for the order of magnitude of the daily amount of the substances for every relevant stage of the life-cycle on the basis of the tonnage. The ranges of the tonnages were typical for substances produced in limited amounts. When the TGD and EUSES were developed these tables were transformed into what are now referred to as the A- and B-tables (A-tables with emission factors and B-tables with size of the operation information) and extended in the following way:

1. extension of the tables with emission factors for several industrial categories. This may be for example for the introduction of main categories or specific use categories. This was also achieved by expert judgement trying to obtain realistic worst-case estimates;
2. insertion of the emission factors of the use category documents mentioned before in the appropriate industrial categories;
3. introduction of B-tables in order to cover higher tonnages for HPVCs (High Production Volume Chemicals). This was also done by expert judgement;
4. new A- and B-tables were developed for the new industrial category 16 'Engineering industries'.

The final tables were discussed and endorsed in a special EU Expert Meeting on Release estimation (Sept. 1995) that was held in the context of the development of the TGD. Subsequently, the tables were introduced in the TGD and EUSES.

13. Calculating releases per stage of the life-cycle

Using the fractions released from the A-tables, the total amount released (per stage of the life-cycle and for each environmental compartment) can be calculated with the following equations. For each stage (except for production) the losses in the previous stage are taken into account.

The fractions released in each stage of the life-cycle and to every compartment are denoted by $F_{i,j}$ where *i* is the stage in the life-cycle and *j* is the compartment:

i	**stage of the life-cycle**	*j*	**compartment**
1	production	a	air
2	formulation	w	water
3	processing	s	soil
4	private use		
5	recovery		

Industrial/professional use is indicated as "processing" in the A- and B-tables. Service life is not included as a separate stage of the life-cycle. With respect to waste disposal, only recovery is addressed in the A- and B-tables.

The release per stage of the life-cycle (in tonnes per year) can be calculated by:

1.

Production	$RELEASE_{1,j}$	air	$F_{1,a}$ • PRODVOL
		water	$F_{1,w}$ • PRODVOL
		soil	$F_{1,s}$ • PRODVOL
		total	$\Sigma F_{1,j}$ • PRODVOL
	amount used:		TONNAGE

2.

Formulation	$RELEASE_{2,j}$	air	$F_{2,a} \cdot TONNAGE$
		water	$F_{2,w} \cdot TONNAGE$
		soil	$F_{2,s} \cdot TONNAGE$
		total	$\Sigma F_{2,j} \cdot TONNAGE$
	rest:		$(1-\Sigma F_{2,j}) \cdot TONNAGE$

3.

Processing	$RELEASE_{3,j}$:	air	$F_{3,a} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		water	$F_{3,w} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		soil	$F_{3,s} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		total	$\Sigma F_{3,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$

4.

Private use	$RELEASE_{4,j}$	air	$F_{4,a} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		water	$F_{4,w} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		soil	$F_{4,s} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		total	$\Sigma F_{4,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		rest:	$(1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$

5.

Recovery	$RELEASE_{5,j}$:	air	$F_{5,a} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		water	$F_{5,w} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		soil	$F_{5,s} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		total	$\Sigma F_{5,j} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$

Explanation of symbols

$F_{i,j}$	Fraction of tonnage released during stage *i* to compartment *j*	[-]	App. IA
PRODVOL	Production volume of the substance	[tonnes · yr^{-1}]	data set
TONNAGE	Tonnage of the substance	[tonnes · yr^{-1}]	eq.(4) (Ch.2)
$RELEASE_{i,j}$	Release during life-cycle stage *i* to compartment *j*	[tonnes · yr^{-1}]	

Abbreviations used in the tables

f	Fraction
HPVC	High Production Volume Chemicals
MC	Main category
IC	Industrial category
Sol.	Solubility (in water) [mg/l]
T	Tonnage [tonnes/year]
UC	Use category
Vap.	Vapour pressure [Pa]

A-tables

Estimates for the emission factors (fractions released)

IC = 1: AGRICULTURAL INDUSTRY

PRODUCTION Table A1.1

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1b	MC=1c	MC=3 1)
Air		<1		0	0	0.00001
		1-10		0	0.00001	0.0001
		10-100		0.00001	0.0001	0.001
		100-1000		0.0001	0.001	0.0
		1000-10,000		0.001	0.005	0.05
		≥10,000		0.005	0.01	0.05
	T (tonnes/year)					
Wastewater	<1000		0.02			
	≥1,000		0.003			
Soil			0.0001			

1) Default

FORMULATION Table A2.1

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1b	MC=1c	MC=3 1)
Air		<10		0.0005	0.001	0.0025
		10-100		0.001	0.0025	0.005
		100-1,000		0.0025	0.005	0.01
		≥1,000		0.005	0.01	0.025
	T (tonnes/year)					
Wastewater	<1,000		0.02			
	≥1,000		0.003			
Soil			0.0001			

1) Default

INDUSTRIAL USE Table A3.1 *

UC's	Description	Emission factors to: Air	Surface water	Soil
Default		0.1	0.1	0.8
3	areosol propellants	1	0	0
9, 10, 36	cleaning/washing agents and additives + colorants + odour agents	0	0.1	0.4
19	fertilisers	0	0.05	0.95
26	food/feedstuff additives	0	0	0.05
38, 50	pesticides + surfactants	0.05	0.1	0.85
41	pharmaceuticals (external application)	0	0	0.1
41	pharmaceuticals (internal application)	0	0	0
48	solvents	1	0	0

* Fertilisers and pesticides + surfactants go to agricultural soil on the regional and continental scale, the others go to industrial soil

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC=2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.2

Conditions		Emission factors		
Sol. (mg/l)	Vap. (Pa)	Air	Wastewater	Soil
<100	<100	0.65	0.25	0.0005
	100-1,000	0.8	0.1	0.0025
	≥1,000	0.95	0.05	0.001
100-1,000	<100	0.4	0.5	0.005
	100-1,000	0.55	0.35	0.002
	≥1,000	0.65	0.25	0.001
1,000-10,000	<100	0.25	0.65	0.005
	100-1,000	0.35	0.55	0.002
	≥1,000	0.5	0.4	0.001
≥10,000	<100	0.05	0.85	0.005
	100-1,000	0.1	0.8	0.002
	≥1,000	0.25	0.65	0.001

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

(Emissions at recovery of chemicals such as catalysts are included in the emissions at industrial use).

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

PRODUCTION Table A1.1 for UC ≠ 33 (intermediates)
Table A1.2 for UC = 33 (intermediates)

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1a	MC=1b	MC=1c
Air		<1		0	0	0
		1-10		0	0	0.00001
		10-100		0	0.00001	0.0001
		100-1,000		0.00001	0.0001	0.001
		1,000-10,000		0.0001	0.001	0.01
		≥10,000		0.001	0.01	0.025
	Process	T (tonnes/year)				
Wastewater	Wet	<1,000	0.02			
		≥1,000	0.003			
	Dry		0			
Soil				0	0.00001	0.0001

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.3

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC = 1b	MC = 1c	MC = 3 (1)
Air		<1		0	0	0.00001
		1-10		0	0	0.0001
		10-100		0	0.00001	0.001
		100-1,000		0.00001	0.0001	0.01
		1,000-10,000		0.0001	0.001	0.025
		≥10,000		0.001	0.005	0.05
	Process	T (tonnes/year)				
Wastewater	Wet	<1,000	0.02			
		≥1,000	0.007	0.0005		
	Dry		0			
Soil			0.0001			

1) Default

Remark: The releases at industrial use for use category 33 (intermediates) should be added to the releases at production **unless** the notifier states that the substance is processed elsewhere.

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.4

Compartment	Conditions Vap. (Pa)	Emission factors MC = 2	MC = 3 [1)]
Air	<100	0.0005	0.0005
	≥100	0.0005	0.001
Wastewater		0.0001	0.005
Soil		0.0001	0.01

1) Default

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 5: PERSONAL /DOMESTIC

PRODUCTION Table A1.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
A1# for UC = 9 and 15 (if production volume < 1,000 tonnes/year Table A1.1 applies)

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors Batch process [1]	Continuous process [2]
Air			0.000 001	0.000 001
Wastewater			[3]	[4]
Solid waste			0	0

[1] e.g., ethoxilation to nonionic surfactants and production of amphoteric and cationic surfactants
[2] e.g., sulphonation and sulphation to anionic surfactants
[3] According to the emission scenario document < 0.3 % (worst case = 0.003)
[4] According to the emission scenario document < 0.1 % (worst case = 0.001)

FORMULATION Table A2.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
Table A2# for UC = 9 (cleaning/washing agents) and UC15 (cosmetics)

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors Regular powder	Compact powder	Liquid	Unknown
Air			0.000 2	0.000 2	0.000 02	0.000 2
Wastewater			0.000 1	0.000 01	0.000 9	0.000 9
Solid waste			0.007 3	0.008 1	0.003 2	0.008 1

INDUSTRIAL USE Not applicable

PRIVATE USE Table A4.1

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Air	2, 7, 8, 9, 10, 11, 15, 41, 47, 50			0
	3			1
	5			0.0005
	26		<5,000	0
			≥5,000	0.01
	35		<5,000	0
			≥5,000	0.05
	36		<100	0.05
			100-2,500	0.2
			2,500-10,000	0.5
			≥10,000	0.9
	38 (herbicides)			0.01
	(pesticides, garden)			0.05
	(pesticides, pets)		<100	0.05
			100-5,000	0.1
			≥5,000	0.8

Table A4.1 continued overleaf

Table A4.1 continued

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Air (cont.)	48, 55	<10	<10 10-100 100-1,000 1,000-10,000 ≥10,000	0.005 0.015 0.15 0.4 0.6
	48, 55	10-100	<10 10-100 100-1,000 1,000-10,000 ≥10,000	0.0015 0.075 0.125 0.25 0.4
	48, 55	100-1,000	<10 10-100 100-1,000 1,000-10,000 ≥10,000	0.0015 0.025 0.1 0.15 0.225
	48, 55	≥1,000	<10 10-100 100-1,000 1,000-10,000 ≥10,000	0.00075 0.03 0.075 0.125 0.175
Surface water	5, 35 (car products)			0.0005
Wastewater	2	25 ≥25		0 0.005
	3, 5, 19, 35 7 8 (household products) (cosmetics)			0 0.01 0.95 0.8
	9, 15 50 10 (cleaning products) (cosmetics) (else)			1 0.99 1 0.8 0.5
	11 26 36 (cosmetics)		 <2,500 2,500-10,000 ≥10,000	0.8 0.025 0.8 0.5 0.1
	(cleaning products,…)		<100 100-2,500 2,500-10,000 ≥10,000	0.9 0.8 0.5 0.1
	(else)		<100 100-2,500 2,500-10,000 ≥10,000	0.5 0.3 0.2 0.05

Table A4.1 continued overleaf

Table A4.1 continued

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Wastewater (cont.)	38 (herbicides) (pesticides, garden) (pesticides, pets)			0 0 0.1
	41 (external) (oral)			0.25 0.05
	47 48, 55		<10 10-100 100-1,000 ≥1,000	0.9 0.1 0.2 0.4 0.6
Soil	2 3, 36, 41 5 7 8 (household products) (cosmetics)			0.0001 0 0.0005 0.001 0.01 0.001
	9, 15 47,50 10 (cleaning products) (cosmetics) (else)			0 0.01 0.002 0.0001 0.01
	11 19 26, 35 38 (garden: herbicides, pesticides) (pesticides, pets)		 <100 100-5,000 ≥5,000	0.0001 1 0.002 0.9 0.05 0.01 0.002
	48, 55		<10 10-100 100-1,000 1,000-10,000 ≥10,000	0.2 0.1 0.05 0.005 0.002

WASTE TREATMENT Not applicable

IC = 6: PUBLIC DOMAIN

PRODUCTION Table A1.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
Table A1# for UC = 9 and 15 (if production volume < 1000 tonnes/year Table A1.1 applies)

FORMULATION Table A2.1 for UC ≠ 9 (cleaning/washing agents)
Table A2# for UC = 9 (cleaning/washing agents)

INDUSTRIAL USE Table A3.5

Conditions Use categories		Emission factors Air	Wastewater	Soil
9	(cleaning/washing agents)			
	≤ 1,000 tonnes/year	0.0025	0.9	0.05
	> 1,000 tonnes/year	0	1	0
39	(non-agric. pesticides)	0.1	0.05	0.8
All	other	0.05	0.45	0.45

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 7: LEATHER PROCESSING INDUSTRY

PRODUCTION Table A1.1 for UC ≠10 (colorants)
Table A1.3 for UC = 10 (colorants)

UC = 10 (Colorants) Compartment	Conditions Sol. (mg/l)	Emission factors
Air		0.0008
Wastewater	<2,000 2,000-10,000 10,000-100,000 100,000-500,000 ≥500,000	0.015 0.02 0.03 0.05 0.06
Soil		0.0001

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.6

Compartment	Conditions Sol. (mg/l)	 Vap. (Pa)	Emission factors All MC's	 MC = 2	 MC = 3 [1)]
Air	<100 <100 ≥100	<100 ≥100	0.001 0.01 0		
Wastewater	<100 100-1,000 ≥1,000			0.05 0.15 0.25	0.9 0.99 0.99
Soil			0.01		

1) Default

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1 for UC ≠ 29 & 35
Table A2.2 for UC = 29 & 35

Compartment	Conditions Vap. (Pa)	Emission factors
Air	<1 1-10 10-100 100-1,000 ≥1,000	0.00005 0.00001 0.0005 0.0025 0.025
Wastewater		0.002
Soil		0.00001

INDUSTRIAL USE Table A3.7

Compartment	Conditions UC≠29&35 Sol. (mg/l)	Emission factors MC = 2	 MC = 3 [1)]
Air		0	0.25
Wastewater	<100 100-1,000 ≥1,000	0.05 0.1 0.25	0.5 0.5 0.5
Soil		0	0.05

Compartment	Conditions UC=29&35 log Henry	Emission factors
Air	<2 ≥2	0.0002 0.002
Wastewater	Pure oils Water based + unknown	0.185 0.316
Soil		0.0001

1) Default

UC 29 = heat transferring agents, UC 35 = lubricants and additives; both are used in metalworking fluids

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.8

Compartment	Conditions Vap. (Pa)	Emission factors
Air	<1	0.0001
	1-10	0.0005
	10-100	0.001
	100-1,000	0.005
	≥1,000	0.01
Wastewater		0.0005
Soil		0.001

PRIVATE USE Table A4.2

Compartment	Conditions Vap. (Pa)	Emission factors
Air	<10	0.005
	10-100	0.015
	100-1,000	0.15
	1,000-10,000	0.4
	≥10,000	0.6
Wastewater		0.0005
Surface water		0.0001
Soil		0.0001

WASTE TREATMENT Not applicable

IC = 10: PHOTOGRAPHIC INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1 default for formulations to be used in photographic baths (aqueous solutions)
Table A2.3 for UC=42, and other UC's in the manufacture of solid materials

Compartment	Conditions Vap. (Pa)	Emission factors
Air	<1 1-10 10-100 100-1,000 ≥1,000	0.0001 0.001 0.3 0.7 1
Wastewater	Control of crystal growth Other functions	0.99 0.002
Soil		0.00025

INDUSTRIAL USE Table A3.9

Compartment	Conditions	Vap. (Pa)	Emission factors MC=2	MC=3 [1)]
Air	Solid materials (e.g. films) Else	 <1 1-10 10-100 100-1,000 ≥1,000	0	 0.000035 0.00025 0.0075 0.025 0.075
Wastewater	Solid materials (e.g. films) Aqueous solutions: - coupler of dye - else		0	 0.15 0.8
Soil	Solid materials (e.g. films) Else		0	 0.00025

1) Default

PRIVATE USE Table A4.3

Compartment	Conditions UC=42 (photochemicals) for aqueous solutions only!	Emission factors
Air		0
Wastewater		0.4
Soil		0

WASTE TREATMENT Table A5.1

Compartment	Conditions UC=42 (photochemicals) for aqueous solutions only! Vap. (Pa)	Emission factors
Air		<10.000005
	1-10	0.000025
	10-100	0.00075
	100-1,000	0.0025
	≥1,000	0.01
Wastewater		0.2
Soil		0

IC = 11: POLYMERS INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.10 for polymerisation processes

In the polymers industry polymers are produced by:

A) Polymerisation reactions: A.1) "Wet" (e.g. emulsion polymerisation)
A.2) "Dry" (e.g. gas phase polymerisation)

B) Other (e.g. polyadditions, polycondensations)

The Use category (HEDSET) for all types of chemicals is: 43 Process regulators, which can be subdivided into:

Type	Type of function
I	Monomers (UC 43 Process regulators)
II	Catalysts (UC 43 Process regulators)
III	Initiators, Inhibitors, Retarders, Chain transfer agents (UC 43 Process regulators), Vulcanising agents (UC 53 Vulcanising agents), etc.

N.B. 1. In principle this might be considered as stage 1. Production!
2. As no good information is available Process types "A" and "B" have been considered to have the same emission factors

Compartment	Conditions	Emission factors					
		Type I		Type II		Type III	
	Vap. (Pa)	"Wet"	"Dry"	"Wet"	"Dry"	"Wet"	"Dry"
Air	<1	0.00001	0.00001	0	0	0	0
	1-10	0.0001	0.0001	0	0	0	0
	10-100	0.001	0.001	0	0	0	0
	100-1,000	0.01	0.01	0.0005	0.0005	0	0
	1,000-10,000	0.05	0.05	0.001	0.001	0.0005	0.0005
	≥10,000	0.05	0.05	0.01	0.01	0.001	0.001
	Sol (mg/l)						
Wastewater	<10	0.00001	0	0.005	0	0.0005	0
	10-100	0.0001	0	0.01	0	0.001	0
	100-1,000	0.001	0	0.025	0	0.0025	0
	≥1,000	0.01	0	0.05	0	0.005	0
	Vap. (Pa)						
Soil	<5,000	0	0	0.0005	0.0005	0.00025	0.00025
	≥5,000	0	0	0	0	0	0

INDUSTRIAL USE Table A3.11 for polymer processing

Processing of polymers ("shaping" by all kind of techniques) occurs in many Industrial categories

Two categories of polymer processing are distinguished:

A	Processing of thermoplastics
B	Processing of thermosetting resins (prepolymers)

For the emission factors the following types of chemicals used are considered:

I	(A, B)	Additives	UC 7 (Anti-static agents), 22 (Flame retardants), 49 (Stabilisers) & 55 Others (e.g. antioxidants)
		Pigments	UC 10 (Colorants)
		Fillers	UC 20
II	(A)	Plasticisers	UC 47 (softeners)
III	(A, B)	Solvents	UC 48
IV	(A, B)	Processing aids	UC 6 (Anti-set off and anti-adhesive agents) & 35 (lubricants and additives)
V	(B)	Curing agents	UC 43 (Process regulators, e.g. initiators)
		Cross-linking agents	UC 43 (Process regulators: monomers)

Compartment	Conditions Vap. (Pa)	Boiling point (°C)	Emission factors A	B	Type of chemicals
Air	<1	<300/unknown	0.001	0	I
		≥300	0.0005	0	
	1-100	<300/unknown	0.0025	0	
		≥300	0.001	0	
	≥100	<300/unknown	0.01	0	
		≥300	0.005	0	
		<400/unknown	0.01		II
		≥400	0.005		
	<100		0.1	0.1	III
	100-1,000		0.25	0.25	
	1,000-10,000		0.5	0.5	
	≥10,000		0.75	0.75	
	<1	<300/unknown	0.01	0	IV
		≥300	0.005	0	
	1-100	<300/unknown	0.025	0	
		≥300	0.01	0	
	≥100	<300/unknown	0.1	0	
		≥300	0.05	0	
	<100			0.075	V
	100-1,000			0.15	
	1,000-10,000			0.25	
	≥10,000			0.35	
Wastewater			0.0005	0.0005	I
			0.001	0	II
			0	0	III
			0.0005	0.0005	IV
				0.00005	V
Soil			0.0001	0.0001	I
			0.0005	0	II
			0.00001	0.00001	III
			0.001	0.001	IV
				0.00001	V

PRIVATE USE Not applicable

WASTE TREATMENT Not considered yet

IC = 12: PULP, PAPER AND BOARD INDUSTRY

PRODUCTION Table A1.1 for UC ≠ 10 (colorants)
Table A1.3 for UC = 10 (colorants)

FORMULATION Table A2.1 for UC ≠ 45 (reprographic agents)
Table A2.1 for UC = 45 (reprographic agents)

INDUSTRIAL USE Table A3.12 for printing and allied processes

Compartment	Conditions Use categories		Emission factors MC = 2	 MC = 3 [1)]
Air	Default	<100 100-1,000 1,000-10,000 ≥10,000	0 0.05 0.25 0.5	0.01 0.2 0.5 0.75
	10 & 45		0	
	48	<100 100-1,000 1,000-10,000 ≥10,000		0.05 0.3 0.65 0.85
		Sol. (mg/l)	MC = 2	MC = 3 [1)]
Wastewater	Default	<100 100-1,000 ≥1,000	0.0001 0.005 0.001	0.01 0.05 0.1
	9			0.9
	10 & 45		0.0005	
	48	<100 100-1,000 ≥1,000		0.0005 0.001 0.005
		Vap. (Pa)	MC = 2	MC = 3 [1)]
Soil	All	<100 100-1,000 1,000-10,000 ≥10,000	0.0015 0.0001 0.00001 0	0.0015 0.0001 0.00001 0

1) Default

INDUSTRIAL USE Table A3.12 for pulp, paper and board production

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors MC=2	MC=3 [1)]
Air	All	<100	<100	0	0.0001
			100-1,000	0.00001	0.001
			≥1,000	0.0001	0.01
		100-1,000	<100	0	0.00001
			100-1,000	0	0.0001
			≥1,000	0.00001	0.001
		≥1,000	<100	0	0
			100-1,000	0	0.0001
			≥1,000	0	0.001
Wastewater	Default	<100	<100	0.85	0.85
			100-500	0.75	0.75
			≥500	0.5	0.5
		100-1,000	<100	0.875	0.875
			100-500	0.85	0.85
			≥500	0.75	0.75
		1,000-10,000	<100	0.9	0.9
			100-500	0.875	0.875
			≥500	0.85	0.85
		≥10,000	-	0.95	0.95
	10:				
	- Basic dye, anion			0.023	0.023
	- Direct dye			0.04	0.04
	- Direct dye, kation			0.055	0.055
	- Direct dye, anion/kation			0.028	0.028
	- Acid dye, kation/unknown			0.079	0.079
	- Brightener			0.064	0.064
	20 & 31			0.05	0.05
Soil	All	<100		0.0015	0.0015
		100-1,000		0.0001	0.0001
		1,000-10,000		0.00001	0.00001
		≥10,000		0	0

1) Default

PRIVATE USE Not applicable

WASTE TREATMENT Table A5.2

Compartment	Conditions	Emission factors
Air		0
Wastewater	Use category = 10 (Colorants)	0.1
	Use category 45, for paper type:	
	- graphic	0.2
	- cardboard	0.01
	- newspaper	0.15
	- sanitary	0.01
	- packing	0.1
	- archives	0.05
	- other, or >1 application	0.2
Soil		0

IC = 13: TEXTILE PROCESSING INDUSTRY

PRODUCTION Table A1.1 for UC ≠ 10 (colorants)
Table A1.3 for UC = 10 (colorants)

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.14

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	UC = 10
Air	<100	<100	0.05	
		100-1,000	0.15	
		≥1,000	0.4	
	100-1,000	<100	0.025	
		100-1,000	0.05	
		≥1,000	0.15	
	1,000-10,000	<100	0.01	
		100-1,000	0.025	
		≥1,000	0.05	
	≥10,000	<100	0.005	
		100-1,000	0.01	
		≥1,000	0.025	
	Batch dyeing			0.0007
	Continuous dyeing			
	- thermosol/unknown			0.05
	- other			0.0025
	- printing			0.0025
Wastewater	<100	<100	0.85	
		100-1,000	0.75	
		≥1,000	0.5	
	100-1,000	<100	0.875	
		100-1,000	0.85	
		≥1,000	0.75	
	1,000-10,000	<100	0.9	
		100-1,000	0.875	
		≥1,000	0.85	
	≥10,000	-	0.95	

Table A3.14 continued overleaf

WASTEWATER for UC = 10 (colorants):
Emission factor (EF) = Emission factor dyeing process (E.1) + Emission factor “handling, washing out and cleaning” (E.2)

$E.1 = A / (1 + K \cdot B)$ B = 1 / liquor ratio (liquor ratio: default = 10 kg fibres / 1 l solution)
A = constant
K = equilibrium constant

INDUSTRIAL USE Table A3.14 Continued

Conditions Type of dye	(**UC = 10**) Type of dyeing	K	A	B	E.2
Disperse	Continuous	115	5	1	0.055
"	Printing	115	2	0.5	0.12
Direct	Batch	73	1	0.1 1)	0.01
Reactive - wool	Batch	190	1	0.1 1)	0.01
Reactive - cotton	Batch	23	1	0.1 1)	0.01
Reactive - general	Batch	57	1	0.1 1)	0.01
Vat	Continuous	190	5	1	0.055
	Printing	190	2	0.5	0.12
Sulphur	Continuous	40	5	1	0.055
	Printing	40	2	0.5	0.12
Acid - one SO3	Batch	90	1	0.1 1)	0.01
Acid - > 1 SO3	Batch	190	1	0.1 1)	0.01
Basic	Batch	990	1	0.1 1)	0.01
Azoic (naphtole)	Continuous	30	5	1	0.055
	Printing	30	2	0.5	0.12
Metal complex	Batch	150	1	0.1 1)	0.01
Pigment	Continuous	5000	5	1	0.055
	Printing	5000	2	0.5	0.12
Unknown, low solubility	Continuous	190	5	1	0.055
	Printing	190	2	0.5	0.12
Unknown, acid groups	Batch	90	1	0.1 1)	0.01

1) Default

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	UC = 10
Soil				0.005
	<100	<100	0.05	
		100-500	0.15	
		≥500	0.4	
	≥100	<100	0.025	
		100-500	0.05	
		≥500	0.15	

PRIVATE USE Table A4.4

Compartment	Conditions Sol. (mg/l)	Emission factors UC<>10	UC=10 1)
Air			0
Wastewater	<250		0.1
	250-1,000		0.15
	1,000-5,000		0.2
	≥5,000		0.3
Soil			0

1) For UC = 10 (Colorants) only, i.e. types used normally by industry for batch dyeing

WASTE TREATMENT Not applicable

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.15

Compartment	Conditions Use category	Vap. (Pa)	Emission factors Water based	Solvent based
Air	3			1
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48		0.8	0.9
		Sol. (mg/l)		
Wastewater	3			0
	10, 14, 20		0.005	0.001
	50	<10	0.005	
		10-100	0.01	
		≥100	0.05	
	47, 52, 55	<10	0.005	0.001
		10-100	0.01	0.005
		≥100	0.05	0.01
	48		0.1	0.02
Soil	3			0
	10, 14, 20		0.005	0.005
	50		0.005	
	47, 52, 55		0.005	0.005
	48		0.001	0.001

PRIVATE USE Table A4.5

Compartment	Conditions Use category	Vap. (Pa)	Emission factors Water based	Solvent based
Air	3			1
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48		0.8	0.95
		Sol. (mg/l)		
Wastewater	3			0
	10, 14, 20		0.005	0.001
	50	<10	0.005	
		10-100	0.01	
		≥100	0.05	
	47, 52, 55	<10	0.005	0.001
		10-100	0.01	0.005
		≥100	0.05	0.01
	48		0.15	0.04
Soil	3			0
	10, 14, 20		0.005	0.005
	50		0.005	
	47, 52, 55		0.005	0.005
	48		0.01	0.01

WASTE TREATMENT Not applicable

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.16

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors MC=2	MC=3 [1)]	MC =4
Air	<100	<10	0.0001	0.001	0.01
		10-100	0.001	0.01	0.1
		100-1,000	0.01	0.1	0.25
		1,000-10,000	0.1	0.5	0.7
		≥10,000	0.5	0.75	0.9
	100-1000	<10	0.00001	0.0001	0.001
		10-100	0.0001	0.001	0.05
		100-1,000	0.001	0.05	0.1
		1,000-10,000	0.05	0.1	0.5
		≥10,000	0.25	0.5	0.75
	≥1,000	<10	0	0.00001	0.0001
		10-100	0.00001	0.0001	0.001
		100-1,000	0.0001	0.001	0.01
		1,000-10,000	0.001	0.01	0.1
		≥10,000	0.01	0.1	0.5
Wastewater	<100	<10	0.01	0.1	0.5
		10-100	0.001	0.01	0.1
		100-1,000	0.0001	0.001	0.01
		1,000-10,000	0.00001	0.0001	0.001
		≥10,000	0	0.00001	0.0001
	100-1000	<10	0.25	0.5	0.75
		10-100	0.05	0.1	0.5
		100-1,000	0.001	0.01	0.1
		1,000-10,000	0.0001	0.001	0.05
		≥10,000	0.00001	0.0001	0.001
	≥1,000	<10	0.5	0.75	0.9
		10-100	0.1	0.5	0.7
		100-1,000	0.01	0.1	0.25
		1,000-10,000	0.001	0.01	0.1
		≥10,000	0.0001	0.001	0.01
Soil	<100	<10	0.005	0.01	0.05
		10-100	0.001	0.005	0.01
		100-1,000	0.0005	0.001	0.005
		1,000-10,000	0	0.0005	0.001
		≥10,000	0	0	0.0005
	100-1000	<10	0.001	0.005	0.01
		10-100	0.0005	0.001	0.005
		100-1,000	0	0.0005	0.001
		1,000-10,000	0	0	0.0005
		≥10,000	0	0	0.0001
	≥1,000	<10	0.0005	0.001	0.005
		10-100	0	0.0005	0.001
		100-1,000	0	0	0.0005
		1,000-10,000	0	0	0.0001
		≥10,000	0	0	0

1) Default

PRIVATE USE Table A3.16

WASTE TREATMENT Not applicable

IC = 0: OTHERS

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.16

B-tables

Estimates for the fraction of the main source and the number of days for emissions

IC = 1: AGRICULTURAL INDUSTRY

PRODUCTION Table B1.1 for new substances and existing substances other than HPVC for UC ≠ 38 & 41

T (tonnes/year)	f main source	No. of days
<1,000	1	0.1f·T
1,000-2,000	0.9	0.1f·T
2,000-4.000	0.75	0.1f·T
≥4,000	0.7	300

PRODUCTION Table B1.2 for new substances and existing substances other than HPVC For UC = 38 & 41

T (tonnes/year)	f main source	No. of days
<10	1	f·T
10-50	0.9	f·T
50-100	0.8	0.6667f·T
100-1,000	0.75	0.4f·T
1,000-2,500	0.6	0.2f·T
≥2,500	0.6	300

PRODUCTION Table B1.3 for HPVC (default ≥10,000) for UC ≠ 38 & 41

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-100,000	0.75	300
>100,000	0.6	300

PRODUCTION Table B1.4 for HPVC (default ≥3,500) for UC = 38 & 41

T (tonnes/year)	f main source	No. of days
<5,000	1	300
5,000-25,000	0.8	300
25,000-100,000	0.6	300
≥100,000	0.4	300

FORMULATION Table B2.1 for new substances and existing substances other than HPVC

T (tonnes/year)	F main source	No. of days
<100	1	2f·T
100-500	0.6	f·T
500-1,000	0.6	0.5f·T
≥1,000	0.4	300

FORMULATION Table B2.2 for HPVC for UC ≠ 38 & 41

T (tonnes/year)	f main source	No. of days
<15,000	1	300
15,000-50,000	0.75	300
≥50,000	0.6	300

FORMULATION Table B2.3 for HPVC for UC = 38 & 41

T (tonnes/year)	f main source	No. of days
<3,500	1	300
3,500-10,000	0.8	300
10,000-25,000	0.7	300
25,000-50,000	0.6	300
≥50,000	0.4	300

INDUSTRIAL USE Table B3.1

T (tonnes/year)	f main source	No. of days for use categories:			
		3,19,39,48,50	41	9,10,36	26
<10	0.05	2	10	50	300
10-100	0.01	2	10	50	300
100-1,000	0.005	2	10	50	300
1,000-10,000	0.001	2	10	50	300
10,000-50,000	0.0005	2	10	50	300
≥50,000	0.00001	2	10	50	300

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION Table B1.1 for non-HPVC
Table B1.5 for HPVC (default ≥10,000)

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-100,000	0.75	300
100,000-500,000	0.6	300
≥500,000	0.5	300

FORMULATION Table B2.4 for non-HPVC
If applicable!

T (tonnes/year)	f main source	No. of days
<10	1	2f·T
10-50	0.9	f·T
50-500	0.8	0.4f·T
500-2,000	0.75	0.2f·T
≥2,000	0.65	300

FORMULATION Table B2.5 for HPVC
If applicable!

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-50,000	0.75	300
≥50,000	0.4	300

INDUSTRIAL USE Table B3.2

T (tonnes/year)	F MAIN SOURCE	NO. OF DAYS
<10	0.8	2f·T
10-50	0.65	f·T
50-500	0.5	0.4f·T
500-2,000	0.4	0.25f·T
2,000-5,000	0.3	0.2f·T
5,000-25,000	0.25	300
25,000-75,000	0.2	300
≥75,000	0.15	300

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

PRODUCTION Table B1.2 for non-HPVC
Table B1.6 for HPVC (default ≥7,000)

T (tonnes/year)	f main source	No. of days
<10,000	1	300
10,000-50,000	0.75	300
50,000-250,000	0.6	300
≥250,000	0.5	300

FORMULATION Table B2.4 for non-HPVC
Table B2.3 for HPVC
If applicable!

INDUSTRIAL USE Table B3.2

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION Table B1.7 for non-HPVC

T (tonnes/year)	f main source	No. of days
<100	1	0.1f · T
100-1,000	0.9	0.1f · T
1,000-2,500	0.8	0.1f · T
≥2,500	0.75	300

PRODUCTION Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.4 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.2

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 5: PERSONAL/DOMESTIC

PRODUCTION Table B1.7 for non-HPVC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.1 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Not applicable

PRIVATE USE Table B4.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
Only for wastewater!

T (tonnes/year)	f main source	No. of days:
	0.002	365

PRIVATE USE Table B4# for UC = 9 and 15 (if production volume < 1,000 tonnes/year Table B4.1 applies)
A) based on tonnage

T (tonnes/year)	No. inhabitants region	No. inhabitants feeding STP	No. of days:
	$2.0 \cdot 10^7$	10,000	365

WASTE TREATMENT Not applicable

IC = 6: PUBLIC DOMAIN

PRODUCTION Table B1.7 for non-HPVC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.1 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.3
Only for wastewater!

T (tonnes/year)	f main source	No. of days for use categories: 9	39	Else
	0.002	200	15	50

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 7: LEATHER PROCESSING INDUSTRY

PRODUCTION Table B1.8 for non-HPVC for UC ≠ 6, 9 10 & 31

T (tonnes/year)	f main source	No. of days
<1,000	1	0.1f·T
1,000-4,000	0.9	0.1f·T
≥4,000	0.75	300

PRODUCTION Table B1.9 for non-HPVC for UC = 6, 9 10 & 31

T (tonnes/year)	f main source	No. of days
<10	1	f·T
10-50	0.9	f·T
50-500	0.5	f·T
500-1,500	0.2	f·T
≥1,500	0.2	300

PRODUCTION Table B1.4 for HPVC (default ≥5,000) for UC ≠ 6, 9 10 & 31
Table B1.4 for HPVC (default ≥2,500) for UC = 6, 9 10 & 31

FORMULATION Table B2.4 for non-HPVC
Table B2.3 for HPVC for UC ≠ 6, 9, 10 & 31
Table B2.6 for HPVC for UC = 6, 9, 10 & 31

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-250,000	0.7	300
≥250,000	0.4	300

INDUSTRIAL USE Table B3.4

T (tonnes/year)	f main source	No. of days
<10	0.8	2f·T
10-50	0.75	2f·T
50-500	0.6	f·T
500-1,500	0.5	0.4f·T
1,500-5,000	0.35	300
5,000-25,000	0.2	300
≥25,000	0.1	300

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

PRODUCTION Table B1.2 for non-HPVC for UC ≠ 29 & 35
Table B1.10 for non-HPVC for UC = 29 & 35

T (tonnes/year)	f main source	No. of days
<10	1	f·T
10-50	0.9	f·T
50-500	0.8	0.6667f·T
500-1,500	0.5	0.4f·T
≥1,500	0.5	300

PRODUCTION Table B1.6 for HPVC (default ≥7,000) for UC ≠ 29 & 35
Table B1.4 for HPVC (default ≥2,500) for UC = 29 & 35

FORMULATION Table B2.4 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.5 for UC = 29 & 35

T (tonnes/year)	No. of days	f main source:	Field of application Primary steelworks	Else
<1,000	300		1	0.8
1,000-5,000	300		0.9	0.5
5,000-50,000	300		0.75	0.3
≥50,000	300		0.6	0.2

INDUSTRIAL USE Table B3.6 for UC ≠ 29 & 35

T (tonnes/year)	f main source	No. of days
<10	1	2f·T
10-50	1	0.5f·T
50-500	0.9	0.4f·T
500-2,000	0.8	0.1875f·T
2,000-10,000	0.7	300
10,000-50,000	0.6	300
≥50,000	0.5	300

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION Table B1.1 for non-HPVC for UC = 27
Table B1.2 for non-HPVC for UC = 28+others
Table B1.4 for HPVC (default ≥3,000) for UC = 28+others
Table B1.11 for HPVC (default ≥25,000) for UC = 27

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-500,000	0.75	300
≥500,000	0.5	300

FORMULATION Table B2.7 for non-HPVC for UC = 27

T (tonnes/year)	f main source	No. of days
<1,000	1	100
1,000-2,000	0.8	200
≥2,000	0.6	300

FORMULATION Table B2.8 for non-HPVC for UC = 28+others

T (tonnes/year)	f main source	No. of days
<5	1	20
5-50	1	60
50-100	1	$2f \cdot T$
100-500	0.8	$f \cdot T$
500-1,000	0.6	$0.5f \cdot T$
≥1,000	0.4	300

FORMULATION Table B2.6 for HPVC for UC = 27
Table B2.6 for HPVC for UC = 28+others

INDUSTRIAL USE Table B3.7

T (tonnes/year)	f main source	No. of days
<50	0.5	350
50-500	0.4	350
500-5,000	0.3	350
5,000-25,000	0.2	350
25000-100,000	0.05	350
≥100,000	0.02	350

PRIVATE USE Table 4.1
Only for wastewater!

WASTE TREATMENT Not applicable

IC = 10: PHOTOGRAPHIC INDUSTRY

PRODUCTION Table B1.4 for HPVC (default ≥4,000)
Table B1.12 for non-HPVC

T (tonnes/year)	f main source	No. of days
<5	1	f·T
5-50	1	0.5f·T
50-250	0.75	0.4f·T
250-3,000	0.5	0.2f·T
≥3,000	0.5	300

FORMULATION Table B2.8 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.8

Company size	f main source	No. of days	
One company	1	300	(No private use)
Large companies	0.333	300	(No private use)
Small companies	0.05	300	

PRIVATE USE Table B4.2
Only for wastewater!
Only if company size at industrial use is small companies (otherwise f main source is zero)

F main source = 0.002·f private use

T (tonnes/year)	f private use	F main source	No. of days:
<10	0	0	200
10-50	0.00002	$4 \cdot 10^{-8}$	200
50-500	0.0001	$2 \cdot 10^{-7}$	200
500-5,000	0.0005	$1 \cdot 10^{-6}$	200
≥5,000	0.0025	$5 \cdot 10^{-6}$	200

WASTE TREATMENT Table B5.1

T (tonnes/year)	f main source	No. of days	One company
<10	1	150	(No private use)
≥10	1	300	

T (tonnes/year)	f main source	No. of days	Large companies
<30	0.333	150	
≥30	0.333	300	

T (tonnes/year)	f main source	No. of days	Small companies
<200	0.2	150	
≥200	0.2	300	

IC = 11: POLYMERS INDUSTRY

PRODUCTION Table B1.9 for non-HPVC for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)
Table B1.13 for non-HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; not: initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<50	0.9	0.4f · T
50-500	0.75	0.2F · T
500-5,000	0.6	0.1f · T
5,000-25,000	0.75	200
≥25,000	0.5	300

PRODUCTION Table B1.4 for HPVC (default ≥3,000) for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)

PRODUCTION Table B1.14 (default ≥60,000) for HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; not: initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-250,000	0.65	300
≥250,000	0.4	300

FORMULATION Table B2.8 for non-HPVC
Table B2.3 for HPVC for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)
Table B2.9 for HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; not: initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-50,000	0.75	300
≥50,000	0.4	300

INDUSTRIAL USE Table B3.9

T (tonnes/year)	f main source	No. of days
<10	0.5	2f · T
10-50	0.35	f · T
50-500	0.25	0.4f · T
500-5,000	0.15	0.4f · T
5,000-25,000	0.1	300
≥25,000	0.05	300

PRIVATE USE Not applicable

WASTE TREATMENT Not considered yet

IC = 12: PULP, PAPER AND BOARD INDUSTRY

PRODUCTION Table B1.8 for non-HPVC for UC ≠ 10 & 45
Table B1.9 for non-HPVC for UC = 10 & 45
Table B1.4 for HPVC (default ≥4,500) for UC ≠ 10 & 45
Table B1.4 for HPVC (default ≥2,500) for UC = 10 & 45

FORMULATION Table B2.1 for non-HPVC for UC ≠ 10 & 45
Table B2.8 for non-HPVC for UC = 10 & 45
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.10

T (tonnes/year)	f main source	No. of days
One company		
<10	1	2f·T
10-50	1	f·T
50-500	1	0.4f·T
≥500	1	300
Large companies		
<100	0.333	2f·T
100-250	0.333	f·T
250-600	0.333	0.5f·T
≥600	0.333	300
Small companies		
<200	0.05	2f·T
200-1,000	0.05	f·T
1,000-6,000	0.05	0.5f·T
6,000-25,000	0.05	300
≥25,000	0.02	300

PRIVATE USE Not considered yet

WASTE TREATMENT Table B5.2

T (tonnes/year)	f main source	No. of days
<100	0.5	150
100-1,000	0.4	200
1,000-10,000	0.3	250
10,000-100,000	0.2	300
≥100,000	0.1	300

IC =13: TEXTILE PROCESSING INDUSTRY

PRODUCTION Table B1.2 for non-HPVC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.3 for HPVC
Table B2.10 for non-HPVC

T (tonnes/year)	f main source	No. of days
<3,500	1	300
3,500-10,000	0.8	300
10,000-25,000	0.7	300
25,000-50,000	0.6	300
≥50,000	0.4	300

INDUSTRIAL USE Table B3.11 for UC = 10

T (tonnes/year)	f main source	No. of days
<10	0.9	10f·T
10-20	0.75	10f·T
20-100	0.6	5f·T
100-1,000	0.4	300
1,000-10,000	0.2	300
≥10,000	0.1	300

INDUSTRIAL USE Table B3.12 for UC ≠ 10

T (tonnes/year)	f main source	No. of days
<10	0.75	5f·T
10-100	0.4	5f·T
100-750	0.4	f·T
750-3,000	0.2	0.5f·T
3,000-25,000	0.2	300
≥25,000	0.1	300

PRIVATE USE Table B4.3
Only for UC = 10 (and only for types of dyes used for batch dyeing by industry)

T (tonnes/year)	f main source	No. of days:
<50	0	
50-500	0.000004	300
≥500	0.00002	300

WASTE TREATMENT Not applicable

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION Table B1.2 for non-HPVC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.10 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.13

T (tonnes/year)	f main source	No. of days
<10	0.9	20f·T
10-50	0.6	6.667f·T
50-300	0.3	3.333f·T
300-5,000	0.15	300
5,000-25,000	0.1	300
≥25,000	0.05	300

PRIVATE USE Table B4.4
Only for wastewater!
Only for paints classified as "do-it-yourself"

F main source = 0.002·f private use

T (tonnes/year)	f private use	f main source	No. of days:
<500	1	0.002	150
≥500	1	0.002	300

PRIVATE USE Table B4.5
Only for wastewater!
Only for paints classified as "constructions, maintenance", etc.

F main source = 0.002·f private use

T (tonnes/year)	f private source	f main source	No. of days:
<50	0	0	
50-500	0.00002	$4 \cdot 10^{-8}$	200
500-2,500	0.0004	$8 \cdot 10^{-7}$	300
2,500-10,000	0.002	$4 \cdot 10^{-6}$	300
10,000-50,000	0.01	$2 \cdot 10^{-5}$	300
≥50,000	0.05	$1 \cdot 10^{-4}$	300

WASTE TREATMENT Not applicable

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION Table B1.2 for non-HPVC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.8 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.14

T (tonnes/year)	f main source	No. of days
<10	1	2f*T
10-50	0.9	f*T
50-500	0.8	0.4f*T
500-2,000	0.75	0.2f*T
2,000-5,000	0.6	0.1f*T
5,000-25,000	0.5	300
≥25,000	0.3	300

PRIVATE USE Table B4.5

WASTE TREATMENT Not applicable

IC = 0 (OTHERS)

PRODUCTION Table B1.2 for non-HPVC
Table B1.6 for HPVC (default ³7,000)

FORMULATION Table B2.8 for non-HPVC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.14

PRIVATE USE Table B4.5

WASTE TREATMENT Table B5.3

T (tonnes/year)	f main source	No. of days
<100	0.5	150
100-1,000	0.3	150
1,000-10,000	0.2	150
≥10,000	0.2	150

Appendix I-a: List of synonyms for functions according to ChemUSES (US EPA, 1980)

No.	Use Category	No.	Function (ChemUSES)
1	Absorbents and adsorbents	131	Absorbents
		60	Adsorbents
		213	Dehumidifiers
2	Adhesive, binding agents	302	Adhesives
		143	Binders
		145	Food additives
		92	Spreaders
		165	Stickers
		280	Tackifiers
3	Aerosol propellants	178	Aerosol propellants
4	Anti-condensation agents		
5	Anti-freezing agents	77	Antifreezes
		74	De-icers
		52	Deodorants
		313	Functional fluids
6	Anti-set-off and anti-adhesive agents	104	Abherents
		63	Antiblocking agents
		188	Anticaking agents
		300	Detackifiers
		233	Dusting agents
		144	Parting agents
		7	Soil retardants
7	Anti-static agents	328	Antistatic agents
		89	Electroconductive coating agents
		318	Humectants
8	Bleaching agents	304	Bleaching assistants
		132	Bleaching agents
9	Cleaning/washing agents and additives	293	Antiredeposition agents
		180	Boil-off assistants
		242	Cleaners
		173	Detergents
		78	Pre-spotting agents
		274	Scouring agents
		261	Shrinkage controllers
		14	Soaping-off assistants
		294	Soil release agents
10	Colouring agents	5	Bloom agents
		86	Colouring agents
		174	Coupling agents (dyes)
		267	Dyes
		20	Fluorescent agents
		248	Lakes
		381	Luminescent agents
		235	Mercerising assistants
		128	Opacifiers
		139	Pearlizing agents
		125	Pigments
		83	Stains

No.	Use Category	No.	Function (ChemUSES)
11	Complexing agents	177	Antiprecipitants
		124	Complexing agents
		10	Sequestering agents
12	Conductive agents	161	Electrical conductive agents
		383	Electrode materials
		245	Electrolytes
		313	Functional fluids
13	Construction materials and additives	324	Case-hardening agents
		355	Concrete additives
		361	Embrittlement inhibitors
		375	Materials for shaping
		250	Reinforcing agents
		349	Water-reducing agents
14	Corrosion inhibitors	230	Antioxidants
		64	Antiscaling agents
		323	Corrosion inhibitors
15	Cosmetics	301	Antiperspirants
		167	Cosmetic ingredients
16	Dust binding agents	26	Dust control agents
17	Electroplating agents	353	Brighteners
		32	Fume suppressants
18	Explosives	179	Detonators
		363	Explosion inhibitors
		158	Explosives
		27	Incendiaries
19	Fertilisers	34	Fertilisers
20	Fillers	351	Fillers (augmentation)
		212	Fillers (patching)
		371	Surface coating additives
		127	Swelling agents
		58	Weighting agents (textile technology)
21	Fixing agents	291	Anticrock agents
		347	Antistripping agents
		268	Barrier coating agents
		295	Fixatives
		134	Fixing agents (fragrances)
		112	Fixing agents (textile technology)
		227	Mordents
22	Flame retardants and fire preventing agents	25	Fire extinguishing agents
		332	Flame retardants
23	Flotation agents	163	Activators (ore processing)
		190	Flocculating agents
		297	Flotation agents
		360	Modifiers
24	Flux agents for casting		
25	Foaming agents	358	Blowing agents
		133	Chemical blowing agents
		94	Frothers
		50	Physical blowing agents

No.	Use Category	No.	Function (ChemUSES)
26	Food/feedstuff additives	214	Acidulants
		66	Feed additives
		80	Sweeteners (taste)
27	Fuels	247	Fuels
28	Fuel additives	329	Antifouling agents
		76	Antiknock agents
		183	Deposit modifiers
		306	Fuel additives
		138	Sweeteners (petroleum technology)
29	Heat transferring agents	72	Coolants
		313	Functional fluids
		199	Heat transfer agents
		216	Quenchers
		208	Refrigerants
30	Hydraulic fluids and additives	313	Functional fluids
		65	Hydraulic fluids
		256	Transmission fluids
31	Impregnation agents	102	Delustrants
		98	Sizes
		258	Water repellents
		23	Waterproofing agents
32	Insulating materials	254	Acoustical insulating material
		311	Electrical insulating material
		314	Heat insulating materials
		162	Insulating materials
33	Intermediates	146	Inorganic intermediates
		115	Monomers
		290	Organic intermediates
		43	Prepolymers
34	Laboratory chemicals	238	Analytical and product testing
		122	Chelating agents
		107	Deionisers
		373	Extraction agents
		69	Indicators
		325	Oxidation-reduction indicators
		374	Reagents
35	Lubricants and additives	119	Antiseize agents
		313	Functional fluids
		148	Internal lubricating agents
		195	Lubricant additives
		364	Lubricating agents
		346	Oiliness agents
		249	Penetrants
		312	Slip agents
36	Odour agents	79	Flavours and fragrances
		339	Odorants

No.	Use Category	No.	Function (ChemUSES)
37	Oxidising agents	149	Oxidisers
38	Plant protection products, agricultural	166	Animal repellents
		333	Bactericides
		108	Biocides
		97	Decontaminats
		270	Fumigants
		362	Fungicides
		275	Herbicides
		155	Insect attractants
		348	Insect repellents
		330	Insecticides
		252	Nematocides
		253	Pesticides
		264	Rodenticides
39	Biocides, non-agricultural	287	Algicides
		1	Antifouling agents
		140	Disinfectants
		118	Preservatives
		116	Slime preventatives
40	PH-regulating agents	172	Laundry sours
		266	pH control agents
		191	pH indicators
41	Pharmaceuticals		
42	Photochemicals	122	Chelating agents
		198	Desensitisers (explosives)
		299	Desensitisers (photography)
		182	Developers
		286	Intensifiers (photography)
		285	Light stabilisers
		344	Photosensitive agents
		303	Sensitisers
43	Process regulators	321	Accelerators
		46	Activators (chemical processes)
		239	Activators (enzymes)
		110	Adhesion promoters
		4	Antifelting agents
		352	Antislip finishing agents
		206	Antistaining agents
		194	Antiwebbing agents
		281	Builders
		222	Carbonising agents
		164	Carriers
		19	Catalyst supports
		170	Catalysts
		31	Chain extenders
		113	Chain terminators
		141	Chain transfer agents
		122	Chelating agents
		114	Coagulants
		278	Coalescents
		357	Coalescing agents

No.	Use Category	No.	Function (ChemUSES)
43	Process regulators (continued)	315	Crabbing assistants
		228	Crosslinking agents
		226	Curing agents (concrete)
		369	Curing agents (polymer technology)
		18	Currying agents
		236	Deasphalting agents
		342	Defoamers
		365	Degumming agents
		137	Dehairing agents
		73	Dehydrating agents
		366	De-inkers
		84	Delignification agents
		30	Depolymerisation agents
		367	Depressants
		292	Desising agents
		259	Dispersants
		317	Dryers
		150	Dye carriers
		255	Dye levelling agents
		307	Dye retardants
		211	Dye retention aids
		341	Enzyme inhibitors
		157	Enzymes
		284	Finishing agents
		337	Formation aids
		331	Fuel oxidisers
		117	Fulling agents
		103	Initiators
		359	Intensifiers (printing)
		171	Kier boiling assistants
		24	Nucleating agents
		96	Peptising agents
		75	Pitch control agents
		121	Polymerisation additives
		209	Polymerisation inhibitors
		21	Prevulcanisation inhibitors
		153	Refining agents
		223	Repulping aids
		136	Retarders
		296	Retention aids
		338	Rubber compounding agents
		51	Scavengers
		326	Solubilising agents
		310	Weighting agents (petroleum technology)
44	Reducing agents	244	Reducers
45	Reprographic agents	225	Toners
46	Semiconductors	202	Semiconductors
		378	Photovoltaic agents
47	Softeners	269	Bates
		231	Devulcanising agents
		28	Elasticisers
		265	Emollients
		185	Plasticisers

No.	Use Category	No.	Function (ChemUSES)
47	Softeners (continued)	29	Softeners
		147	Water softeners
48	Solvents	229	Degreasers
		82	Dewaxing solvents
		373	Extraction agents
		320	Paint and varnish removers
		16	Reaction media
		271	Solvents
49	Stabilisers	277	Anticracking agents
		12	Antifume agents
		129	Antihydrolysis agents
		168	Antiozonants
		230	Antioxidants
		120	Antilivering agents
		282	Antiplasticisers
		160	Antisagging agents
		68	Antisettling agents
		88	Bloom inhibitors
		123	Coupling agents (polymers)
		159	Emulsifiers
		87	Heat stabilisers
		54	Stabilisers
		36	Ultraviolet absorbers
50	Surface-active agents	41	Antifloating agents
		234	Antifogging agents
		109	Surfactants
		243	Wetting agents
51	Tanning agents	316	Tanning agents
52	Viscosity adjustors	152	Antiflooding agents
		120	Antilivering agents
		343	Antiskinning agents
		221	Gelling agents
		262	Pour point depressants
		272	Thickeners
		334	Thixotropic agents
		240	Turbulence suppressors
		135	Viscosity adjustors
		15	Viscosity index improvers
53	Vulcanising agents	288	Vulcanising agents
54	Welding and soldering agents	101	Brazing agents
		22	Fluxing agents
0	Other	204	Ablatives
		105	Abrasives
		196	Activators (luminescence)
		354	Aerating agents
		47	Air entraining agents
		376	Alloying agents
		90	Anticratering agents
		48	Anticreasing agents
		99	Antifogging agents

No.	Use Category	No.	Function (ChemUSES)
0	Other (continued)	218	Antipilling agents
		350	Antiskid agents
		6	Blasting abrasives
		70	Bluing agents
		220	Bright dips
		93	Chemical raw materials
		298	Clarifiers
		260	Cloud point depressants
		130	Coating agents
		283	Collectors
		335	Coupling agents (solutions)
		215	Culture nutrients
		81	Deaerating agents
		309	Deblooming agents
		85	Dechlorinating agents
		73	Dehydrating agents
		107	Deionisers
		232	Demulsifiers
		200	Denaturants
		49	Descaling agents
		205	Dewatering aids
		356	Discharge printing agents
		38	Drainage aids
		44	Drilling mud additives
		322	Dry strength additives
		39	Dye stripping agents
		100	Electron emission agents
		340	Eluting agents
		372	Embalming agents
		186	Encapsulating agents
		57	Enhanced oil recovery agents
		308	Entraining agents
		319	Etching agents
		336	Evaporation control agents
		373	Extraction agents
		207	Fiber-forming compounds
		368	Filtration aids
		56	Flatting agents
		79	Flavours and fragrances
		142	Fluid loss additives
		313	Functional fluids
		193	Greaseproofing agents
		184	“Grinding, lapping, sanding and”
		192	Hormones
		246	Humidity indicators
		210	Hydrotropic agents
		181	Impact modifiers
		380	Incandescent agents
		69	Indicators
		2	Ion exchange agents
		91	Lachrymators
		33	Latex compounding agents
		53	Leaching agents
		156	Leather processing agents
		370	Liquid crystals
		381	Luminescent agents

No.	Use Category	No.	Function (ChemUSES)
		379	Magnetic agents
		67	Mar proofing agents
		289	Metal conditioners
		95	Metal strippers
		37	Metal treating agents
		327	Milling aids
		237	Obscuring agents
		197	Oil repellents
		62	Optical quenchers
		382	Osmotic membranes
		17	Papermaking agents
		55	Phosphatising agents
		203	Phosphorescent agents
		59	Pickling agents
		217	Pickling inhibitors
		251	Plant growth regulators
		176	Plastics additives
		224	Plastics for shaping
		169	Plating agents
		8	Poison gas decontaminants
		3	Polymer strippers
		111	Pore forming agents
		151	Precipitating agents
		106	Protective agents
		45	Radioactivity decontaminants
		374	Reagents
		219	Refractive index modifiers
		241	Refractories
		154	Resists
		9	Rinse aids
		71	Ripening agents
		187	Rubber for shaping
		201	Rubber reclaiming agents
		189	Rubbing fastness agents
		276	Rust inhibitors
		11	Rust removers
		263	Scrooping agents
		42	Sealants
		98	Sizes
		126	Slime control agents
		305	Soil conditioners
		61	Strippers
		40	Tar removers
		345	Tarnish inhibitors
		13	Tarnish removers
		279	Textile specialities
		257	Vat printing assistants
		273	Wax strippers
		35	Well treating agents
		175	Wet strength additives
		377	X-ray absorbents

Appendix I-b: List of synonyms for functions according to ChemUSES (US EPA, 1980)

No.	ChemUSES Function	Use category EU (No.)
104	Abherents	6
204	Ablatives	55
105	Abrasives	0
131	Absorbents	1
321	Accelerators	43
214	Acidulants	26
254	Acoustical insulating material	32
46	Activators (chemical processes)	43
163	Activators (ore processing)	23
196	Activators (luminescence)	55
239	Activators (enzymes)	43
110	Adhesion promoters	43
302	Adhesives	2
60	Adsorbents	1
354	Aerating agents	0
178	Aerosol propellents	3
47	Air entraining agents	0
287	Algicides	39
376	Alloying agents	0
238	Analytical and product testing	34
166	Animal repellents	38
63	Antiblocking agents	6
188	Anticaking agents	6
277	Anticracking agents	49
90	Anticratering agents	0
48	Anticreasing agents	0
291	Anticrock agents	21
4	Antifelting agents	43
41	Antifloating agents	50
152	Antiflooding agents	52
234	Antifogging agents	50
99	Antifogging agents	0
1	Antifouling agents	39
329	Antifouling agents	28
77	Antifreezes	5
12	Antifume agents	49
129	Antihydrolysis agents	49
76	Antiknock agents	28
120	Antilivering agents	49, 52
230	Antioxidants	14, 49
168	Antiozonants	49
301	Antiperspirants	15
218	Antipilling agents	55
282	Antiplasticisers	49
177	Antiprecipitants	11
293	Antiredeposition agents	9
160	Antisagging agents	49
64	Antiscaling agents	14
119	Antiseize agents	35
68	Antisettling agents	49
350	Antiskid agents	0
343	Antiskinning agents	52
352	Antislip finishing agents	43
206	Antistaining agents	43
328	Antistatic agents	7
347	Antistripping agents	21
194	Antiwebbing agents	43
333	Bactericides	38
268	Barrier coating agents	21
269	Bates	47
143	Binders	2
108	Biocides	38
6	Blasting abrasives	0
132	Bleaching agents	8
304	Bleaching assistants	8
5	Bloom agents	10
88	Bloom inhibitors	49
358	Blowing agents	25
70	Bluing agents	0
180	Boil-off assistants	9
101	Brazing agents	54
220	Bright dips	0
353	Brighteners	17
281	Builders	43
222	Carbonising agents	43
164	Carriers	43
324	Case-hardening agents	13
170	Catalysts	43
19	Catalyst supports	43
31	Chain extenders	43
113	Chain terminators	43
141	Chain transfer agents	43
122	Chelating agents	34, 42, 43
133	Chemical blowing agents	25
93	Chemical raw materials	0
298	Clarifiers	0
242	Cleaners	9
260	Cloud point depressants	0
114	Coagulants	43
278	Coalescents	43
357	Coalescing agents	43
130	Coating agents	0
283	Collectors	0
86	Colouring agents	10
124	Complexing agents	11
355	Concrete additives	13
72	Coolants	29
323	Corrosion inhibitors	14
167	Cosmetic ingredients	15
123	Coupling agents (polymers)	49
174	Coupling agents (dyes)	10
335	Coupling agents (solutions)	55
315	Crabbing assistants	43
228	Crosslinking agents	43
215	Culture nutrients	0
226	Curing agents (concrete)	43
369	Curing agents (polymer technology)	43
18	Currying agents	43
366	De-inkers	43
81	Deaerating agents	0
236	Deasphalting agents	43
309	Deblooming agents	0
85	Dechlorinating agents	55
97	Decontaminats	38
342	Defoamers	43
229	Degreasers	48
365	Degumming agents	43
137	Dehairing agents	43
213	Dehumidifiers	1
73	Dehydrating agents	0, 34
74	Deicers	5
107	Deionizers	0, 34
84	Delignification agents	43
102	Delustrants	31
232	Demulsifiers	0
200	Denaturants	0
52	Deodorants	5
30	Depolymerisation agents	43

183	Deposit modifiers	28
367	Depressants	43
49	Descaling agents	0
198	Desensitisers (explosives)	42
299	Desensitisers (photography)	42
292	Desizing agents	43
300	Detackifiers	6
173	Detergents	9
179	Detonators	18
182	Developers	42
231	Devulcanising agents	47
205	Dewatering aids	0
82	Dewaxing solvents	48
356	Discharge printing agents	0
140	Disinfectants	39
259	Dispersants	43
38	Drainage aids	0
317	Dryers	43
44	Drilling mud additives	0
322	Dry strength additives	0
26	Dust control agents	16
233	Dusting agents	6
150	Dye carriers	43
255	Dye leveling agents	43
307	Dye retardants	43
211	Dye retention aids	43
39	Dye stripping agents	0
267	Dyes	10
28	Elasticisers	47
161	Electrical conductive agents	12
311	Electrical insulating material	32
89	Electroconductive coating agents	7
383	Electrode materials	12
245	Electrolytes	12
100	Electron emission agents	0
340	Eluting agents	0
372	Embalming agents	0
361	Embrittlement inhibitors	13
265	Emollients	47
159	Emulsifiers	49
186	Encapsulating agents	0
57	Enhanced oil recovery agents	0
308	Entraining agents	0
341	Enzyme inhibitors	43
157	Enzymes	43
319	Etching agents	0
336	Evaporation control agents	0
363	Explosion inhibitors	18
158	Explosives	18
373	Extraction agents	34, 48
66	Feed additives	26
34	Fertilisers	19
207	Fiber-forming compounds	0
212	Fillers (patching)	20
351	Fillers (augmentation)	20
368	Filtration aids	0
284	Finishing agents	43
25	Fire extinguishing agents	22
295	Fixatives	21
112	Fixing agents (textile technology)	21
134	Fixing agents (fragrances)	21
332	Flame retardants	22
56	Flatting agents	0
79	Flavours and fragrances	0, 36
190	Flocculating agents	23
297	Flotation agents	23
142	Fluid loss additives	0
20	Fluorescent agents	10
22	Fluxing agents	54
145	Food additives	2
337	Formation aids	43
94	Frothers	25
306	Fuel additives	28
331	Fuel oxidisers	43
247	Fuels	27
117	Fulling agents	43
32	Fume suppressants	17
270	Fumigants	38
313	Functional fluids	0, 5, 12, 29, 30, 35
362	Fungicides	38
221	Gelling agents	52
193	Greaseproofing agents	0
184	Grinding, lapping, sanding and polishing abrasives	0
99	Heat transfer agents	29
314	Heat insulating materials	32
87	Heat stabilisers	49
275	Herbicides	38
192	Hormones	0
318	Humectants	7
246	Humidity indicators	0
65	Hydraulic fluids	30
210	Hydrotropic agents	0
181	Impact modifiers	0
380	Incandescent agents	0
27	Incendiaries	18
69	Indicators	0, 34
103	Initiators	43
146	Inorganic intermediates	33
155	Insect attractants	38
348	Insect repellents	38
330	Insecticides	38
162	Insulating materials	32
286	Intensifiers (photography)	42
359	Intensifiers (printing)	43
148	Internal lubricating agents	35
2	Ion exchange agents	0
171	Kier boiling assistants	43
91	Lachrymators	0
248	Lakes	10
33	Latex compounding agents	0
172	Laundry sours	40
53	Leaching agents	0
156	Leather processing agents	0
285	Light stabilisers	42
370	Liquid crystals	0
195	Lubricant additives	35
364	Lubricating agents	35
381	Luminescent agents	0, 10
379	Magnetic agents	0
67	Mar proofing agents	55
375	Materials for shaping	13
35	Mercerising assistants	10
289	Metal conditioners	0
37	Metal treating agents	0
95	Metal strippers	0
327	Milling aids	0
360	Modifiers	23
115	Monomers	33
227	Mordents	21
252	Nematocides	38
24	Nucleating agents	43
237	Obscuring agents	0
339	Odorants	36
197	Oil repellents	0
346	Oiliness agents	35
128	Opacifiers	10
62	Optical quenchers	0

290	Organic intermediates	33
382	Osmotic membranes	0
325	Oxidation-reduction indicators	34
149	Oxidisers	37
320	Paint and varnish removers	48
17	Papermaking agents	0
144	Parting agents	6
139	Pearlising agents	10
249	Penetrants	35
96	Peptising agents	43
253	Pesticides	38
191	pH indicators	40
266	pH control agents	40
55	Phosphatising agents	0
203	Phosphorescent agents	0
344	Photosensitive agents	42
378	Photovoltaic agents	42
50	Physical blowing agents	25
217	Pickling inhibitors	0
59	Pickling agents	0
125	Pigments	10
75	Pitch control agents	43
251	Plant growth regulators	0
185	Plasticisers	47
176	Plastics additives	0
224	Plastics for shaping	0
169	Plating agents	0
8	Poison gas decontaminants	0
3	Polymer strippers	0
121	Polymerisation additives	43
209	Polymerisation inhibitors	43
111	Pore forming agents	0
262	Pour point depressants	52
78	Pre-spotting agents	9
151	Precipitating agents	0
43	Prepolymers	33
118	Preservatives	39
21	Prevulcanisation inhibitors	43
106	Protective agents	0
216	Quenchers	29
45	Radioactivity decontaminants	0
16	Reaction media	48
374	Reagents	0, 34
244	Reducers	44
153	Refining agents	43
219	Refractive index modifiers	0
241	Refractories	0
208	Refrigerants	29
250	Reinforcing agents	13
223	Repulping aids	43
154	Resists	0
136	Retarders	43
296	Retention aids	43
9	Rinse aids	0
71	Ripening agents	0
264	Rodenticides	38
338	Rubber compounding agents	43
187	Rubber for shaping	0
201	Rubber reclaiming agents	0
189	Rubbing fastness agents	0
11	Rust removers	0
276	Rust inhibitors	0
51	Scavengers	43
274	Scouring agents	9
263	Scrooping agents	0
42	Sealants	0
202	Semiconductors	46
303	Sensitisers	42
10	Sequestering agents	11
261	Shrinkage controllers	9
98	Sizes	0, 31
126	Slime control agents	0
116	Slime preventatives	39
312	Slip agents	35
14	Soaping-off assistants	9
29	Softeners	47
305	Soil conditioners	0
294	Soil release agents	9
7	Soil retardants	6
326	Solubilising agents	43
271	Solvents	48
92	Spreaders	2
54	Stabilisers	49
83	Stains	10
165	Stickers	2
61	Strippers	0
371	Surface coating additives	20
109	Surfactants	50
138	Sweeteners (petroleum technology)	28
80	Sweeteners (taste)	26
127	Swelling agents	20
280	Tackifiers	2
316	Tanning agents	51
40	Tar removers	0
13	Tarnish removers	0
345	Tarnish inhibitors	0
279	Textile specialities	0
272	Thickeners	52
334	Thixotropic agents	52
225	Toners	45
256	Transmission fluids	30
240	Turbulence suppressors	52
36	Ultraviolet absorbers	49
257	Vat printing assistants	0
135	Viscosity adjustors	52
15	Viscosity index improvers	52
288	Vulcanising agents	53
147	Water softeners	47
258	Water repellents	31
349	Water-reducing agents	13
23	Waterproofing agents	31
273	Wax strippers	0
310	Weighting agents (petroleum technology)	43
58	Weighting agents (textile technology)	20
35	Well treating agents	0
175	Wet strength additives	0
243	Wetting agents	50
377	X-ray absorbents	0

Appendix I-c: Input scheme for emission data on substances

1. Characterisation

	Yes	No
High production volume chemical	☐	☐
Other existing chemical	☐	☐
New chemical	☐	☐
Not specified	☐	

2. Tonnage

A Produced (tpa): ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐

B Imported (tpa): ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐

C Exported (tpa): ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐

3. Use and stages of the life-cycle

	Yes	No
Production	☐	☐

		Processing			Production		Formulation		Private use		Recovery	
No.	Fraction	IC	UC	No	Yes	No	Yes	No	Yes	No	Yes	No
1	☐ ☐ ☐	**5**	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
2	☐ ☐ ☐	☐ ☐	☐ ☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
3	☐ ☐ ☐	☐ ☐	☐ ☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
4	☐.☐ ☐	☐ ☐	☐ ☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
5	☐.☐ ☐	☐ ☐	☐ ☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

N.B. Private use is specified by IC 5 Personal/Domestic; This is the direct use of the substance (or a formulation containing the substance) by the public at large.
If the processing step has not to be considered at the assessment "No" is marked (not applicable for IC 5).

4. Production characteristics

D Main producer (tpa): ☐,☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐

Not specified: ☐

IC 3, UC 33

Non-isolated intermediate	(MC 1a)	☐
Isolated intermediate, stored on site	(MC 1b)	☐
Isolated intermediate with controlled transport	(MC 1c)	☐
Not specified	(MC 1c)	☐

Other IC/UC combinations

Continuous production	(MC 1b)	☐
Batch process with dedicated equipment	(MC 1c)	☐
Batch process with multi-purpose equipment	(MC 3)	☐
Not specified	(MC 3)	☐

Production capacity of the main source (producer)

E Capacity (t/day)	☐ ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐
F Period (days/year)	☐ ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐
Not specified	☐

Specific emission information

Emission	**G**: kg/tonne	**or**	Fraction (**EFcomp-prod**)
Air	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Wastewater	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Soil	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Not specified	☐		

5. Formulation characteristics

N.B. For every IC/UC-combination specified in (3) Use and stage of the life-cycle:

Specific information on the scale of formulation

One company (fraction of main source = 1)	☐
Fraction of main source (**Fms-form**)	0. ☐ ☐ ☐
specified	☐

No specific emission information

Dedicated equipment and (very) little cleaning operations	(MC 1b)	☐
Dedicated equipment and frequent cleaning operations	(MC 1c)	☐
Multi-purpose equipment	(MC 3)	☐
Unknown		☐

Specific emission information

Emission	**H**: kg/tonne	**or**	Fraction (**EFcomp-form**)
Air	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Wastewater	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Soil	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐

Content in formulated product

Content:	☐ ☐ ☐. ☐ ☐ ☐ %, or fraction:	0. ☐ ☐ ☐

In case of a given range:

Minimum:	☐ ☐ ☐. ☐ ☐ ☐ %, or fraction:	0. ☐ ☐ ☐
Maximum:	☐ ☐ ☐. ☐ ☐ ☐ %, or fraction:	0. ☐ ☐ ☐

6. Processing characteristics

N.B. **For every IC/UC-combination specified in (3) Use and stage of the life-cycle:**

Information on the scale of processing

One company (fraction of main source **Fms-proc** = 1)	☐
Fraction of main source (**Fms-proc**)	0. ☐ ☐ ☐
Not specified	☐

Specific emission information

Emission	**I**: kg/tonne	**or**	Fraction (**EFcomp-proc**)
Air	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Wastewater	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Soil	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐

N.B. For every IC/UC-combinations specific data will be asked to input for release scenarios based on emission scenario documents!

7. Private use characteristics

Specific emission information

Emission	**J**: kg/tonne	**or**	Fraction (**EFcomp-priv**)
Air	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Wastewater	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Soil	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐

8. Recovery characteristics

Specific information on the scale of recovery

Fraction of product (containing the substance)/substance recovered	0. ☐ ☐ ☐
Fraction recovered by the main source	0. ☐ ☐ ☐

Specific emission information

Emission	**K**: kg/tonne	**or**	Fraction (**EFcomp-rec**)
Air	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Wastewater	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Soil	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐

Appendix II Fate of chemicals in a wastewater treatment plant based on the SimpleTreat model

The tables in this appendix provide values for the fate of substances that enter the sewage treatment plant, estimated according to the SimpleTreat 3.0 model (Struijs et al., 1996). The tables provide information on how much of a substance that enters the sewage treatment plant goes to air, surface water and to sewage sludge and how much is degraded. Separate tables are given depending on the categorization of a substance according to the results of screening biodegradation tests (see Table 6).

The data in the tables have been obtained from calculations with the SimpleTreat 3.0 model with the following settings: the volume of wastewater is set at 200 l per capita per day in line with Table 9 (Section 2.3.7.1). Assuming that the total amount of solids in raw sewage produced per inhabitant per day is $0.150\ (m^{-3} \cdot d^{-1}) \cdot 0.6\ (kg \cdot m^{-3})$ = 90 g per inhabitant per day, the concentration of suspended matter in influent has been set to $0.45\ (kg \cdot m^{-3})$ (see Table 9). In order to maintain the main characteristics of the sludge flow, the steady-state concentration of suspended solids in the primary settler has been set at 150 mg dry weight per l, implying that still 2/3 of the solids in raw sewage is separated by the primary settler. Consequently, settled sewage flowing from the primary settler into the aeration tank contains an oxygen requirement (R_o) of 176 mg BOD per l.

The mode of operation is defined by the input parameter sludge loading rate which specifies the BOD loading of the plant. The operation of the activated sludge reactor is largely specified by this parameter. This input parameter is in units of kg BOD per kg dry weight per day and is related to the sludge retention time (SRT) or sludge age and the hydraulic retention time (HRT). A medium sludge loading rate of 0.15 kg BOD $kg_{dw}^{-1} \cdot d^{-1}$ is used with a SRT of 9.2 d and an HRT of 7.1 hr.

Compared to previous versions of the model in SimpleTreat 3.0 a correction for stripping chemicals has been included, as the process description is only valid for volatile chemicals (H > 250 $Pa \cdot m^3 \cdot mol^{-1}$). The overall mass transfer coefficient during surface aeration (k_{surf}) was assumed proportional to the dissolved oxygen overall transfer rate coefficient ($K_L a_O$), estimated from the oxygen requirement (R_o), hydraulic retention time (HRT) and the difference between the oxygen saturation and the actual O_2 concentration in the aerator (ΔO_2). In order to account also for the gas phase resistance (H < 250 $Pa \cdot m^3 \cdot mol^{-1}$) the proportionality constant Ψ, still having the default value of 0.6, should be multiplied by a factor containing the dimensionless Henry constant (K_H) and the ratio of the mass transfer rate coefficients of a chemical in air and water. Munz and Roberts (1987) recommend to apply 40 as a default value for this ratio. As a result the first order rate constant for surface aeration is written as:

$$k_{surf} = \psi \left(\frac{40 \cdot K_H}{40 \cdot K_H + 1}\right) \frac{R_O}{HRT \cdot \Delta O_2}$$

In the following tables H (Henry's law constant) should be used in $Pa \cdot m^3 \cdot mol^{-1}$.

a) No biodegradability

Fate of chemicals that are not degradable: $kbio_{stp}$ = 0 hr^{-1} in the aqueous phase of activated sludge.

		log H									
	% to air	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	2	15	64	91	95	95
	1	0	0	0	0	2	15	64	91	95	95
	2	0	0	0	0	2	15	64	91	94	95
	3	0	0	0	0	2	14	62	89	92	92
	4	0	0	0	0	1	12	52	77	80	80
	5	0	0	0	0	1	5	28	48	51	51
	6	0	0	0	0	0	1	9	23	27	27

		log H									
	% to water	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	100	100	100	100	98	85	36	9	5	5
	1	100	100	100	100	98	85	36	9	5	5
	2	99	99	99	99	97	84	36	9	5	5
	3	96	96	96	96	94	82	35	8	5	5
	4	79	79	79	79	77	68	30	8	5	4
	5	39	39	39	39	39	35	19	6	4	4
	6	15	15	15	15	15	14	11	6	4	4

		log H									
	% to sludge	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
	3	4	4	4	4	4	4	3	3	3	3
	4	21	21	21	21	21	20	18	16	15	15
	5	61	61	61	61	60	59	53	46	45	45
	6	85	85	85	85	85	85	80	71	69	69

		log H									
	% degraded	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	0	0	0	0	0	0	0	0	0	0
	3	0	0	0	0	0	0	0	0	0	0
	4	0	0	0	0	0	0	0	0	0	0
	5	0	0	0	0	0	0	0	0	0	0
	6	0	0	0	0	0	0	0	0	0	0

		log H									
	% removal	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	2	15	64	91	95	95
	1	0	0	0	0	2	15	64	91	95	95
	2	1	1	1	1	3	16	64	91	95	95
	3	4	4	4	4	6	18	65	92	95	95
	4	21	21	21	21	23	32	70	92	95	96
	5	61	61	61	61	61	65	81	94	96	96
	6	85	85	85	85	85	86	89	94	96	96

b) Inherent biodegradability

Fate of chemicals that are "inherently biodegradable" in an OECD/EU test: $kbio_{stp} = 0.1\ hr^{-1}$ in the aqueous phase of activated sludge.

		log H									
	% to air	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	1	10	50	85	91	91
	1	0	0	0	0	1	10	50	85	91	91
	2	0	0	0	0	1	10	50	85	90	91
	3	0	0	0	0	1	9	49	83	88	89
	4	0	0	0	0	1	8	41	72	77	77
	5	0	0	0	0	0	4	23	45	49	49
	6	0	0	0	0	0	1	8	22	26	26

		log H									
	% to water	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	59	59	59	59	58	52	28	8	5	5
	1	59	59	59	59	58	52	28	8	5	5
	2	59	59	59	59	58	52	27	8	5	5
	3	57	57	57	57	56	50	27	8	5	5
	4	48	48	48	48	48	43	24	7	5	4
	5	28	28	28	28	27	25	16	5	4	3
	6	13	13	13	13	13	13	10	6	4	4

		log H									
	% to sludge	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
	3	4	4	4	4	4	4	3	3	3	3
	4	19	19	19	19	19	19	17	16	15	15
	5	56	56	56	56	56	55	51	46	45	45
	6	83	83	83	83	82	82	78	71	69	68

		log H									
	% degraded	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	41	41	41	41	41	38	22	7	4	4
	1	41	41	41	41	40	38	22	7	4	4
	2	41	41	41	41	40	38	22	7	4	4
	3	39	39	39	39	39	37	21	6	4	4
	4	33	33	33	33	32	31	18	6	4	3
	5	17	17	17	17	16	16	10	4	2	2
	6	4	4	4	4	4	4	4	2	1	1

		log H									
	% removal	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	41	41	41	41	42	48	72	92	95	95
	1	41	41	41	41	42	48	72	92	95	95
	2	41	41	41	41	42	48	73	92	95	95
	3	43	43	43	43	44	50	73	92	95	95
	4	52	52	52	52	52	57	76	93	95	96
	5	72	72	72	72	73	75	84	95	96	97
	6	87	87	87	87	87	87	90	94	96	96

c) pass levels within 28 days in a test on "ready biodegradability", 10-day window criterion is not fulfilled

Fate of chemicals that reach the biodegradation pass levels within 28 days in an OECD/EU test on "ready biodegradability but not within the 10 day time window: $kbio_{stp}$ = 0.3 hr^{-1} in the aqueous phase of activated sludge.

		log H									
	% to air	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	1	6	36	76	84	85
	1	0	0	0	0	1	6	36	76	84	85
	2	0	0	0	0	1	6	36	75	83	84
	3	0	0	0	0	1	6	35	73	81	82
	4	0	0	0	0	1	5	30	64	71	71
	5	0	0	0	0	0	3	17	40	45	46
	6	0	0	0	0	0	1	7	20	24	25

		log H									
	% to water	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	33	33	33	33	32	29	19	7	5	4
	1	33	33	33	33	32	29	19	7	5	4
	2	32	32	32	32	32	29	19	7	5	4
	3	32	32	32	32	31	29	18	7	5	4
	4	27	27	27	27	27	25	16	6	4	4
	5	18	18	18	18	17	16	12	5	3	3
	6	11	11	11	11	11	10	9	5	4	4

		log H									
	% to sludge	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
	3	3	3	3	3	3	3	3	3	3	3
	4	17	17	17	17	17	17	16	16	15	15
	5	51	51	51	51	51	51	49	46	45	45
	6	79	79	79	79	79	78	76	70	68	68

		log H									
	% degraded	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	67	67	67	67	67	64	45	17	12	11
	1	67	67	67	67	67	64	45	17	12	11
	2	67	67	67	67	67	64	45	17	12	11
	3	65	65	65	65	65	62	44	17	11	11
	4	55	55	55	55	55	53	38	15	10	9
	5	31	31	31	31	31	30	22	9	6	6
	6	11	11	11	11	11	10	9	5	3	3

		log H									
	% removal	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	67	67	67	67	68	71	81	93	95	96
	1	67	67	67	67	68	71	81	93	95	96
	2	68	68	68	68	68	71	81	93	95	96
	3	68	68	68	68	69	71	82	93	95	96
	4	73	73	73	73	73	75	84	94	96	96
	5	82	82	82	82	83	84	88	95	97	97
	6	89	89	89	89	89	90	91	95	96	96

d) pass levels within 28 days in a test on "ready biodegradability", 10-day window criterion is fulfilled

Fate of chemicals that are "readily biodegradable" in an OECD/EU test: $kbio_{stp}$ = 1 hr^{-1} in the aqueous phase of activated sludge.

		log H									
	% to air	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	3	19	55	66	68
	1	0	0	0	0	0	3	19	55	66	68
	2	0	0	0	0	0	3	19	54	66	67
	3	0	0	0	0	0	3	18	53	64	66
	4	0	0	0	0	0	3	16	46	56	57
	5	0	0	0	0	0	1	9	29	36	37
	6	0	0	0	0	0	1	4	15	20	20

		log H									
	% to water	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	13	13	13	13	13	12	9	5	4	3
	1	13	13	13	13	13	12	9	5	4	3
	2	13	13	13	13	12	12	9	5	4	3
	3	12	12	12	12	12	11	9	5	4	3
	4	11	11	11	11	11	10	8	4	3	3
	5	8	8	8	8	8	7	6	4	3	3
	6	7	7	7	7	7	7	6	4	3	3

		log H									
	% to sludge	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	0	0	0	0	0	0	0	0	0	0
	3	3	3	3	3	3	3	3	3	3	3
	4	16	16	16	16	16	16	16	15	15	15
	5	47	47	47	47	47	47	46	45	45	45
	6	72	72	72	72	72	72	71	69	67	67

		log H									
	% degraded	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	87	87	87	87	87	85	72	41	30	29
	1	87	87	87	87	87	85	72	40	30	29
	2	87	87	87	87	87	85	72	40	30	29
	3	85	85	85	85	84	82	70	39	29	28
	4	73	73	73	73	73	71	61	34	26	24
	5	45	45	45	45	45	44	38	22	17	16
	6	21	21	21	21	21	21	19	12	9	9

		log H									
	% removal	-4	-3	-2	-1	0	1	2	3	4	5
log Kow	0	87	87	87	87	87	88	91	95	96	97
	1	87	87	87	87	87	88	91	95	96	97
	2	87	87	87	87	88	88	91	95	96	97
	3	88	88	88	88	88	89	91	95	96	97
	4	89	89	89	89	89	90	92	96	97	97
	5	92	92	92	92	92	93	94	96	97	97
	6	93	93	93	93	93	93	94	96	97	97

Appendix III Evaluation of data

In determining whether or not the data to be used in the risk assessment are adequate, their quality and representativeness needs to be evaluated. For this, a number of factors will be considered and the test design will be evaluated to ensure that the quality criteria demanded by standardised tests have in part or in whole been met. Such quality criteria can be detailed in general terms but expert judgement will be required for each substance and test data on a case-by-case basis. A number of papers address the issue of data quality (e.g. SIDS Manual (OECD, 1994a); AQUIRE-database-manual; Tema Nord, 1994). Care should be taken that the guidance given is appropriate for the use of data. The following factors should be taken into account when evaluating the data (on aquatic toxicity):

Identity of the test substance

It is important that the substance tested be properly identified and any significant impurities described. Ideally, this should be through the quoting of a CAS No. or other substance specific means but the substance name may often be sufficient. However, tests conducted on "dichloro....." when the substance being evaluated is "1,3-dichloro....." may thus be insufficient to determine exactly what substance was tested. Equally, the presence or absence of a significant toxic impurity may affect the measured toxicity. Where such an impurity is identified in the substance under evaluation, due care should be taken to ensure that its effects are fully taken into account.

Test organisms

Detailed information of the taxonomic identity of aquatic organisms tested should be supplied, to include the genus and species. While tests on "non-standard" organisms can be accepted, care should be taken to ensure that they are properly characterised and the test system appropriate. The animals should be of relatively uniform age, weight and size and should be healthy at the start of test as shown by low mortality/effects in controls.

Test design

The test system should be adequately described and be considered appropriate for the substance of concern and organisms tested. The delivery of the test substance should be ensure a controlled and known exposure and the supply of oxygen, food and light be suitable to reduce unnecessary stress in the test organisms. The temperature, pH and water hardness should be recorded and be appropriate for the organisms tested. The number of organisms exposed and number of exposure concentrations chosen should be sufficient for a valid statistical calculation of the appropriate effects concentrations to be made.

- the delivery of the test substance represents a critical stage in ensuring adequate exposure of the test organisms. When considering the delivery system, due account should be taken of the relevant phys. chem. properties of the test substance and their potential effects on the delivery and exposure systems. For Daphnia and algae static tests are normally used but for fish static, semi-static or flow-through tests may be appropriate. The precise mechanism used to deliver the test substance must therefore be described;
- the exposure concentration should be known and maintained under control (>80% of initial concentrations) throughout the test. Ideally, the concentrations should be directly measured at appropriate stages over the course of the test. In many cases, measured concentrations will

not be available and expert judgement will be necessary to decide whether the exposure of the aquatic organisms is adequately described. Such non-measured concentrations are normally described as 'nominal' concentrations and refer to the level at which it was intended that exposure would occur. Such concentrations may be acceptable if the test substance:

- is sufficient soluble in test water, i.e. the test concentrations are below the water solubility;
- is relatively stable in test water;
- has a low absorbance to the system delivery and exposure apparatus;
- is non-volatile.

For the interpretation of data that were generated by using solubilisers the altered bioavailability (enhancement/reduction) has to be considered. For many substances, including poorly water soluble substances, volatile substances and substances that hydrolyse or adsorb on surfaces, nominal concentrations are often not appropriate and additional information may be necessary in order to verify the actual exposure concentrations. In some cases, the choice of a semi-static or flow-through system (fish test) may allow a presumption of a stable exposure concentration. In general, the more likely it is that the physical chemical properties of the substance would lead to a loss of concentration over the course of the test, the more important it becomes to verify the concentration by direct analysis of the test water at suitable points throughout the test. Where the exposure concentration can not be determined with confidence, the test should be regarded as ' not-valid' for the purposes or risk assessment;

- The environmental conditions which exist during the test should be recorded and be both stable and appropriate. Significant variations in the environmental conditions such as pH, temperature, water hardness, oxygen levels and light regime can induce undue stress within the test organisms and hence false levels of toxicity. Absence of information on these parameters would suggest that the test system was not well described although would not necessary invalidate the data if other quality criteria are met;

- The L(E)C50 would normally be determined on a statistical basis from the effects observed over a range of concentrations. It is important, therefore, that sufficient organisms are tested at each concentration level and sufficient concentration levels are chosen so as to allow a statistically valid derivation to be made of the appropriate effect concentration. In the absence of this details, a clear indication of the method used to calculate the effect (or no effect) concentration may be sufficient. Limit tests would not normally be acceptable expect as a means of demonstrating no toxic effects;

- At issue is whether the duration of a standard toxicity test(s) is long enough for the compound to reach steady state and elicit a toxic response (Hawker and Connell, 1985; Connell, 1990; Kristensen and Tyle 1990). For many organic non-metabolizable compounds, the time to reach respectively 80% and 95% of the steady state concentration is depending on lipophilicity of the compound (OECD, 1994b).

Field studies

In general field studies are difficult to interpret. Touart (1988) developed guidance criteria for aquatic mesocosm tests with pesticides. Emans et al. (1993) used a set of criteria to assess the quality of field studies. This set can serve as a tool for evaluation:

1. a distinct concentration-effect relationship should be obtained,
2. a reliable MS NOEC should be derived,
3. several taxonomic groups, in more or less natural ecosystems, should be exposed to one test concentration for a longer period,
4. in each experiment several concentrations should be tested, consisting of one control and at least two test concentrations,
5. each test concentration should have at least one replica,
6. the concentration of the test compound should be measured several times during the experiment,
7. physico-chemical parameters like pH, temperature and hardness should be measured,
8. apart from effect parameters like population density and biomass also effect parameters on higher integration levels such as species diversity and species richness should be measured.

References

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Appendix IV Assignment of organisms to trophic levels

Primary producers

Primary producers photo-/chemo-autotrophically synthesise organic compounds using inorganic precursors. They include:

- chlorophyll-containing species of vascular plants
- algae, (e.g. green algae: *Selenastrum*, *Scenedesmus*, *Chlorella*; blue-green algae: *Microcystis*)
- purple sulphur bacteria, chlorobacteria
- chemoautotrophic bacteria (nitrifying bacteria, sulphur bacteria).

Primary consumers

They live mainly on living or dead autotrophic organisms or on microorganisms. Representatives of this trophic level are especially plant-eating animals (i.e. species that are not carnivorous of the following taxonomic groups):

- protozoa (e.g. *Uronema, Entosiphon, Tetrahymena*)
- annelida (e.g. *Tubifex, Enchytraeus*)
- crustacea (e.g. *Artemia, Daphnia* spec., *Copepoda, Gammarus, Asellus*)
- molluscs (e.g. *Dreissena, Mytilus, Ostrea*; several gastropods: *Patella, Viviparus*)
- insects (some insect larvae that are not carnivorous)
- nematoda (those species which are living in water)

Secondary consumers

They live mainly on primary consumers. Among them are:

- predatory insects and larvae of insects (e.g. *Chaoborus*)
- carnivorous protozoa
- rotatoria
- coelenterata (e.g. *Hydra*)
- predatory copepods
- fish (*Teleostei*: e.g. *Cyprinus carpio*, *Brachydanio rerio*, *Poecilia reticulata*, *Oryzias latipes*, *Pimephales promelas*, *Lepomis macrochirus*, *Oncorhynchus mykiss* (previously: *Salmo gairdneri*, *Leuciscus idus melanotus*, *Cyprinodon*, *Carassius*)
- amphibians (e.g. *Rana, Xenopus*)

Decomposers

Organisms of this trophic level break down dead organic material to inorganic constitu-ents.

Standard organisms are underlined

Organisms used in ecotoxicological tests can be assigned to different trophic levels, taxonomic groups, life forms (e.g. sessil, planktonic or swimming), and feeding strategies (e.g. autotrophic, carnivorous, herbivorous, detritivorous, scavengers, omnivorous, deposit or filter feeders.) These assignments are related to differences in morphology, behaviour, and physiology, including their ability to take up, metabolise and excrete chemicals. Furthermore, these assignments may also to some extent determine the likelihood, extent and way the organisms may be exposed. Taken

together the mentioned differences may explain the observed variability among organisms regarding their sensitivity to the toxicity of chemicals, even though it may be difficult or impossible to attribute which differences between two organisms are the actual reason for their sensitivity to a certain toxic chemical.

The standard organisms which are usually used in standard tests (plankton micro-algae, Daphnia and fish) represent three trophic levels (primary producers, primary consumers and secondary consumers), three taxonomic groups (green algae, crustaceans and bone fish), two life forms (plankton or nekton) and three feeding strategies (photosynthetic, herbivorous filter feeder and carnivorous).

Accordingly, non-standard organisms can be assigned to equivalent trophic levels, taxonomic groups etc.

The assignment of an organism to a trophic level is based on the energy balance of the ecosystem concerned and is not primarily dependent on the species. Therefore, a given population may represent more than one trophic level depending on the spectrum and amount of nutrition for the species. In addition, earlier life stages may live on completely different nutrition compared to adults of the same species.

Appendix V Examples of assays suitable for further testing for soil organisms

Soil organisms

A few suitable test species belonging to additional taxonomic groups were identified in the SERAS-Workshop in 1992 (Soil Ecotoxicological Risk Assessment System). Van Straalen and Van Gestel (1992), Stavola (1990) and Samsøe-Petersen and Pedersen (1994) discuss a number of terrestrial species and test methods with various degrees of standardisation. Léon and Van Gestel (1994) give possible criteria for the evaluation of individual tests and for the selection of standardised laboratory toxicity tests with terrestrial organisms.

Results obtained in tests carried out in accordance with guidelines for pesticides may pose a problem. Only tests where the test substance is applied to the soil in a comparable way to the exposure of existing chemicals can be used for the concentration-effect assessment. Following recognition of the lack of standardised soil tests, research programmes have been initiated in Sweden (MATS = MArk Test System), in the Netherlands (NISRP = Netherlands Integrated Soil Research Programme) and in Denmark.

A co-ordinated programme for the development and standardisation of a number of soil test species and test systems has also been initiated. This project SECOFASE (Sub-lethal Effects of Chemicals On FAuna Soil Ecosystem) is described by Løkke and Van Gestel (1993, cited in Samsøe-Petersen and Pedersen (1994)). It should be noted that the guideline for a long-term test with vascular plants has still to be finalised (e.g. with *Arabidopsis thaliana* or *Brassica rapa*, Stavola (1990)). Long-term tests for the earth- and compost worms (ISO draft, 1993; Dutch Draft Guideline; German Draft Guideline), and the test on Enchytraeids, OECD new guideline 220, draft March 2000), and the spring-tail (Dutch Draft Guideline; German Draft; BBA 1990b) are available. These tests analyse effects on reproduction. In addition, the standardisation of the long-term test on Staphylinids (*Coleoptera*), where degree of parasitism, hatching rate and reproduction are assessed, is close to completion (Samsøe-Petersen, 1987; Naton, 1989; SETAC, 1995).

For biocidal active substances, the Technical Notes for Guidance on data requirements in support to Directive 98/8/EC proposes guidance to the additional data requirements in case further testing are necessary after the results of the ecotoxicological studies submitted in the common core data set and the intended use(s) of the active substance, as well as further testing strategies for evaluating the fate and behaviour in the environment of the active substance together with its transformation products and their ecotoxicological effects (TNsG on Data Requirements, 2000).

Table 1 Selected soil test methodologies

Test Organism	Duration	Endpoints	Reference/Source	Comments
Microbial Processes				
Microbial Processes N-Transformation	≥28 d	M	(i) EU draft C.21: Soil Microorganisms. Nitrification Transformation Test. (ii) OECD 216 Soil Microorganisms, Nitrogen Transformation Test (2000). (iii) ISO 14238 Soil quality – Biological methods: Determination of nitrogen mineralisation and nitrification in soils and the influence of chemicals on these processes (1997).	– Addresses short-term adverse effects. – Based on soil microflora nitrate production. – Bacteria are present at up to 10 million per cm^2 in soils. This corresponds to several tonnes per hectare.
Microbial Processes C-Transformation	≥28 d	M	(i) EU draft C.22: Soil Microorganisms. Carbon Transformation Test. (ii) OECD 217 Soil Microorganisms, Carbon Transformation Test (2000). (iii) ISO 14238 Soil quality – Laboratory incubations systems for measuring the mineralisation of organic chemicals in soil under aerobic conditions (1997).	– Addresses short-term adverse effects. – Based on soil microflora respiration rate. – Bacteria are present at up to 10 million per cm^2 in soils. This corresponds to several tonnes per hectare.
Invertebrate Fauna				
Eisenia fetida/andrei (Oligochaeta)	7 – 14 d	S	(i) EU C.8: Earthworm acute toxicity test. (ii) OECD 207 Earthworm acute toxicity tests (1984). (iii) ISO 11268-1 Soil Quality – Effects of pollutants on earthworms (*Eisenia fetida*). Part 1: Determination of acute toxicity using artificial soil substrate (1993). (iv) ASTM E1676-97 Standard guide for conducting laboratory soil toxicity or bioaccumulation tests with the Lumbricid earthworm *Eisenia fetida* (1997).	– Adult survival assessed after 1 – 2 weeks. – Important ecological function (enhance decomposition and mineralisation via incorporation of matter into soil). – Important food source and potential route of bioaccumulation by higher organisms. – Large size/ease of handling. – Readily cultured/maintained in the laboratory. – Litter-dwelling epigeic species. – Standard test organism for terrestrial ecotoxicology. – The Lumbricidae account for 12% of the edaphon (soil biota) by biomass and are therefore important prey species.

Table 1 continued overleaf

Table 1 continued Selected soil test methodologies

Test Organism	Duration	Endpoints	Reference/Source	Comments
Invertebrate Fauna (continued)				
Eisenia fetida/andrei (Oligochaeta)	28d + 28d	S/G/R	(i) OECD (2000). Earthworm Reproduction Test (Draft). (ii) ISO 11268-2 Soil Quality – Effects of Pollutants on Earthworms (*Eisenia fetida*). Part 2: Determination of Effects on Reproduction (1998). (iii) US EPA (1996). Ecological Effects Test Guidelines. OPPTS 850.6200 Earthworm Subchronic Toxicity Test. US EPA, Prevention, Pesticides and Toxic Substances (7104). EPA712-C-96-167, April 1996. (iv) Kula & Larink (1998). Tests on the earthworms *Eisenia fetida* and *Aporrectodea caliginosa*. **In** Handbook of Soil Invertebrates (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Adult growth and survival assessed after 4 weeks. – Reproduction (juvenile number) assessed after a further 4 weeks (8 weeks total). – Relatively long generation time (8 weeks). – Important ecological function (enhance decomposition and mineralisation via incorporation of matter into soil). – Important food source and potential route of bioaccumulation by higher organisms. – Large size/ease of handling. – Readily cultured/maintained in the laboratory. – Litter-dwelling epigeic species. – Standard test organism for terrestrial ecotoxicology. – The Lumbricidae account for 12% of the edaphon (soil biota) by biomass and are therefore important prey species.
Aporrectodea caliginosa (Oligochaeta)		S/G/R	Kula & Larink (1998). Tests on the earthworms Eisenia fetida and Aporrectodea caliginosa. **In** Handbook of Soil Invertebrates (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Mortality, growth and cocoon number assessed after 4 weeks. – Relatively slow reproductive cycle. – Cultures difficult to maintain. – Horizontal burrowing (endogeic) mineral soil species. – Selective feeders digesting fungi, bacteria and algae. – Dominant in agro-ecosystems. Present at 10 – 250 per m^2.

Table 1 continued overleaf

Table 1 continued Selected soil test methodologies

Test Organism	Duration	Endpoints	Reference/Source	Comments
Invertebrate Fauna (continued)				
Enchytraeus albidus (Oligochaeta)	21 - 42d	S/R	(i) OECD (2000). OECD 220 Enchytraeidae Reproduction Test (Draft). (ii) ISO/CD 16387 Soil quality - Effects of soil pollutants on enchytraeids: Determination of effects on reproduction (draft).	– Adult mortality is assessed after 3 weeks. – Reproduction (juvenile number) is assessed after a further 3 weeks (6 weeks total). – Shorter generation time than earthworms. – Ease of handling/culture. – Enchytraeidae feed on decomposing plant material and associated microorganisms i.e., fungi, bacteria & algae. – Enchytraeids are abundant in many soil types including those from which earthworms are often absent. They account for approximately 0.5% of the edaphon (soil biota) by mass (up to 50 g per m^2). This corresponds to approximately 100,000 per m^2.
Cognettia sphagnetorum (Oligochaeta)	70 d	G/R	Rundgren & Augustsson (1998). Test on the Enchytraeid Cognettia sphagnetorum. **In** Handbook of Soil Invertebrates (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Mortality and asexual reproduction (fragmentation rate of adults) determined weekly over 10 weeks. – Easy to culture. – Enchytraeidae feed on decomposing plant material and associated microorganisms i.e., fungi, bacteria & algae. – C. spagnetorum is common in bogs, forests and other highly organic habitats. They are present at 10,000 – 25,000 per m^2.
Folsomia candida (Collembola)	28d	S/R	ISO 11267 Soil Quality – Inhibition of reproduction of Collembola (Folsomia candida) (1999).	– Survival and reproduction after 4 weeks. – Short generation time. – Ease of culture. – Springtails are important soil litter arthropods playing a role in soil organic matter breakdown and nutrients recycling. – Feed on bacteria and fungi. – Collembola are the most abundant soil fauna present at 40,000 to 70,000 per m^2. Prey for epigeic invertebrates such as mites, centipedes, spiders and carabid beetles.

Table 1 continued overleaf

Table 1 continued Selected soil test methodologies

Test Organism	Duration	Endpoints	Reference/Source	Comments
Invertebrate Fauna (continued)				
Isomtoma viridis, Folsomia candida and Folsomia fimetaria (Collembola)	28 - 56 d	S/G/R	Willes & Krogh (1998). Tests with the Collembolans Isomtoma viridis, Folsomia candida and Folsomia fimetaria. **In** Handbook of Soil Invertebrates (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Survival and reproduction assessed weekly (cf. ISO protocol). – Dermal and alimentary uptake. – Springtails are important soil litter arthropods playing q role in soil organic matter breakdown and nutrients recycling. – Feed on bacteria and fungi. – The most abundant soil fauna present at 10,000 to 50,000 per m^2. Prey for epigeic invertebrates such as mites, centipedes, spiders and carabid beetles.
Hypoaspis Aculieifer (Gamasid mite) preying on *Folsomia Fimetaria* (Collembola)	21 d	S/G/R	Krogh & Axelson (1998). Test on the predatory mite *Hypoaspis Aculieifer* preying on the Collembolan *Folsomia Fimetaria*. **In** Handbook of Soil Invertebrates (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Mortality, growth and offspring number assessed after three weeks. – Natural prey-predator relationship. – Predacious species feeding on enchytraeids, nematodes and micro-arthropods. Important role in control of parasitic nematodes. – Gamasioda mites are present at 5 - 10,000 per m^2.
Porcellio scaber (Isopoda)	28 – 70 d	S/G/R	Hornung et al. (1998). Tests on the Isopod *Porcellio scaber*. In "*Handbook of Soil Invertebrates*" (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Survival and biomass determined after 4 weeks (weekly measurements). – Reproduction (oocyte number, % gravid females, % females releasing juveniles, number offspring) determined after 10 weeks. – Alimentary uptake via dosed food or soil. – Isopods woodlouse species. Macro-decomposers important part of detritus food chain. – Important prey species for centipedes. – Estimated population density of isopods is 500 – 1,500 per m^2.

Table 1 continued overleaf

Table 1 continued Selected soil test methodologies

Test Organism	Duration	Endpoints	Reference/Source	Comments
Invertebrate Fauna (continued)				
Brachydesmus superus (Diplopoda)	70 d	S/R	Tajovsky (1998). Test on the Millipede Brachydesmus superus. In "Handbook of Soil Invertebrates" (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Animal number, nest number, egg number and offspring number determined weekly. – Difficult to maintain culture throughout year. – Alimentary uptake via dosed food or soil. – Millipedes are important primary decomposers of leaf litter and organic detritus. – Their faecal pellets provide a micro-environment for microorganisms such as fungi and micro-arthropods. – Important prey for carabid beetles, centipedes and spiders and insectivorous birds and mammals. Diplopoda are present at 10 – 100 per m^2.
Lithobius mutabilis (Chilopoda)	28 – 84 d	S/G/L/M	Laskowski et al. (1998). Test on the Centipede Lithobius mutabilis. In "Handbook of Soil Invertebrates" (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Mortality, biomass, respiration rate and locomotor activity determined after 4 weeks (degradable compounds) to 12 weeks (persistent compounds). – Food chain effect measured via use of dosed prey (fly larvae). – Centipedes are important carnivorous arthropods feeding on small earthworms, millipedes, woodlice and springtails. They are in turn prey for birds and mammals. Chilopoda are present up to 100 per m^2.
Philonthus cognatus (Coleoptera)	42 – 70 d	S/R	Metge & Heimbach (1998). Test on the Staphylinid Philonthus cognatus. In "Handbook of Soil Invertebrates" (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Beetles exposed for one week to determine subsequent effect on egg production and hatching rate over 6 – 10 weeks. Mortality may also be assessed. – Predators of springtails, aphids, dipterans & coleopteran larvae. Prey to birds, mice and large arthropods. – Estimated densities of 1 adult per 2 – 5 m^2.

Table 1 continued overleaf

Table 1 continued Selected soil test methodologies

Test Organism	Duration	Endpoints	Reference/Source	Comments
Invertebrate Fauna (continued)				
Competition between *Plectus acuminatus* (Nematoda) and *Heterocephalobus pauciannulatus* (Nematoda)	14 d	S/R	Kammenga & Riksen (1998). Test on the competition between the nematodes Plectus acuminatus and Heterocephalobus pauciannulatus. **In** Handbook of Soil Invertebrates (Eds. Hans Løkke & Cornelis A.M. Van Gestel). John Wiley & Sons: Chichester, UK.	– Competition between two bacterivorous nematode species. – Ratio determined after two weeks. – Nematodes are important in decomposition and cycling of organic materials. – Abundant and readily retrieved from soil and cultured. – Nematodes are the most abundant element of the mesofauna and account for 2% by mass of the edaphon (soil biomass). This corresponds to approximately 10 million per m^2.
Caenorhabditis elegans (Nematoda)	1 d	S	(i) Donkin & Dusenbury (1993). A soil toxicity test using the nematode Caenorhabditis elegans and an effective method of recovery. Arch. Environ. Contam. Toxicol. 25, 145-151. (ii) Freeman et al. (1999). A soil bioassay using the nematode Caenorhabditis elegans. ASTM STP 1364. (iii) Peredney & Williams (2000). Utility of Caenorhabditis elegans for assessing heavy metal contamination in artificial soil. Arch. Environ. Contam. Toxicol. 39, 113-118.	– Mortality assessed after 1 d. – Important in decomposition and cycling of organic materials. – Abundant and readily retrieved from soil and cultured. – Nematodes are the most abundant element of the mesofauna and account for 2% by mass of the edaphon (soil biomass). This corresponds to approximately 10 million per m^2 or 1 g per m^2.
Caenorhabditis elegans (Nematoda)	3d	G/R	(i) Neumann-Hensel & Ahlf (1998). Deutsche Bundesstiftung Umwelt Report Number 05446. (ii) Höss (2001). Bestimmung der Wirkung von Sediment- und Bodenproben auf Wachstum und Fruchtbarkeit von Caenorhabditis elegans (Nematoda). Draft DIN standard.	– Growth and reproduction assessed after 3 days. – Abundant and readily retrieved from soil and cultured. – Sublethal bioassay (high survival is a pre-requisite for test validity). – Nematodes are the most abundant element of the mesofauna and account for 2% by mass of the edaphon (soil biomass). This corresponds to approximately 10 million per m^2 or 1 g per m^2.

Table 1 continued overleaf

Table 1 continued Selected soil test methodologies

Test Organism	Duration	Endpoints	Reference/Source	Comments
Primary Producers				
Many test species including grass crops (monocotyledonae - Gramineae), Brassica spp. (Dicotyledonae – Cruciferae) and bean crops (Dicotyledonae – Leguminosae)	5d or 14 – 21 d	E/G	(i) OECD (2000). OECD 208A Seedling emergence and seedling growth test & OECD 208B: Vegetative vigour test (draft). (ii) ISO 11269-1: Soil quality – Determination of the effects of pollutants on soil flora – Part 1: Method for the measurement of inhibition of root growth (1993). (iii) ISO 11269-2 Soil quality – Determination of the effects of pollutants on soil flora – Part 2: Effects of chemicals on the emergence and growth of higher plants (1995). (iv) ASTM E1963-98 Standard guide for conducting terrestrial plant toxicity tests (1998).	– Seed emergence (E) & early life stages of growth (G) in treated soils (208A) – Vegetative vigour (G) following foliar application (208B). – Root growth of pre-germinated seeds (ISO 11269-1). – Minimum of three test species: one monocotyledon and two dicotyledon (OECD 208,)

Key: S = survival; E = emergence; G = growth; R = reproduction; M = metabolism; L = locomotory activity

Appendix VI Examples of assays suitable for futher testing for sediment organisms

In the table selected freshwater sediment toxicity test methods are presented (adapted from SETAC, 1993). Further sediment tests, e.g. for marine species, can be found in OECD (1998a).

Table 1 Selected freshwater sediment toxicity test methodologies (adapted from SETAC, 1993)

Test organism	Duration	Endpoints	Reference	Comments
Chironomus sp. (Insect)	28d	S/E	ASTM (1994). Standard Guide for Conducting Sediment Toxicity Tests with Freshwater Invertebrates (E-1383-94a). ASTM: Philadelphia OECD GL 218 (draft) and 219 (draft)	- short generation time - larvae in direct contact with sediment by burrowing - filter feeder / surface deposit feeder - supplementary feeding required* - wide tolerance of sediment grain size - important prey organisms
Hexagenia sp. (Insect)	21d	S/G	ASTM (1994). Standard Guide for Conducting Sediment Toxicity Tests with Freshwater Invertebrates (E-1383-94a). ASTM: Philadelphia	- nymphs in direct contact with sediment by burrowing - surface particle collector - fine / organically enriched sediments
Lumbriculus variegatus (Oligochaete)	28d	S/G/R	Phipps et al. (1993): Use of the aquatic oligochaete Lumbriculus variegatus for assessing the toxicity and bioaccumulation of sediment-associated contaminants. Env. Tox. Chem. 12, 269-279	- short generation time - subsurface deposit feeder - inhabits a wide variety of sediment types
Tubifex tubifex (Oligochaete)	28d	S/R	(1) Reynoldson et al. (1991): A sediment bioassay using the Tubificid Oligochaete worm Tubifex tubifex. Env. Tox. Chem. 10, 1061-1072. (2) ASTM (1994): Standard Guide for Conducting Sediment Toxicity Tests with Freshwater Invertebrates (E-1383-94a). ASTM: Philadelphia	- short generation time - subsurface deposit feeder - tolerant of variation in sediment particle size and proportion organic matter - important ecological link in aquatic food chain and active in bioturbation
Hyalella azteca (Amphipod)	30d	S/G/R	ASTM (1994). Standard Guide for Conducting Sediment Toxicity Tests with Freshwater Invertebrates (E-1383-94a). ASTM: Philadelphia	- short generation time - some subsurface deposit feeding - supplementary feeding required* - wide tolerance of sediment grain size

Table 1 continued overleaf

Table 1 continued Selected freshwater sediment toxicity test methodologies (adapted from SETAC, 1993)

Test organism	Duration	Endpoints	Reference	Comments
Gammarus sp. (Amphipod)	> 28 d	S/F	Pascoe et al. (1992): Development and validation of methods for evaluating chronic toxicity to freshwater ecosystems. Final Summary Report of the Environmental Research Programme Assessment of Risk Associated with Chemicals (Ecotoxicology). EEC RTD Contract EV4V-0110-UK(BA)	- long generation time (R possible at > 3 month) - limited growth when not fed - supplementary feeding required* - epibenthic detrivore - sensitive to sediment size (fine sediments are not a suitable habitat)
Diporeia sp. (Amphipod)	28d	S	ASTM (1994). Standard Guide for Conducting Sediment Toxicity Tests with Freshwater Invertebrates (E-1383-94a). ASTM: Philadelphia	- long generation time and slow growth - subsurface deposit feeder - relatively insensitive to grain size
Caenorhabditis elegans (Nematode)	3d	G/R	(1) Traunspurger et al. (1997): Ecotoxicological assessment of aquatic sediments with Caenorhabditis elegans (Nematoda) – A method for testing liquid medium and whole-sediment samples. Env. Tox. Chem. 16, 245-250. (2) Höss et al. (1997): Influence of particle size distributions and content of organic matter on the toxicity of copper in sediment bioassays using Caenorhabditis elegans (Nematoda). Water, Air and Soil Pollution 99, 689-695	- short life-cycle - sublethal bioassay (high survival is preriquisite for test validity) - infaunal bacterial ingester - Bacteria (E. coli) suspensions added as a food source prior to introduction of nematodes to test vessels - sensitive to particle size distribution (ingestion of fine particles reduces relative quantity of bacteria in diet) - nematodes are the most abundant /Species rich metazoans in sediments

Key: S = survival, E = emergence, G = growth, R = reproduction, F = feeding

* Tests with species that need supplementary feeding should be designed in such a way that the food taken up by the test organisms is also contaminated with the test substance. This is necessary to adequately address the exposure to the test substance via ingestion

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Appendix VII Toxicity data for fish-eating birds and mammals

The endpoints of the tests should be expressed as a concentration in food (mg test substance/kg food). Often test results for birds and mammals are expressed in mg/kg body weight/day. These data should be converted to a concentration in food (mg/kg). For the conversion, data on body weight and daily food intake during the tests need to be known. This conversion is only advisable when no other toxicity data for birds and mammals are available. If this information cannot be obtained from the test report, the values on body weight, daily food intake and daily water intake that are given in the table can be used for the transformation. For transformation of toxicity data expressed on the basis of body weight or water intake to food intake, the toxicity data should be multiplied by the conversion factor (BW/DFI or DWI/DFI).

Table 1 Conversion factors for toxicity data (Sax, 1989; Romijn et al., 1993)

	BW	DFI	DWI	BW/DFI	DWI/DFI
Canis domesticus	10,000	250		40	
Macaca spec.	5,000	250		20	
Microtus spec.	25	3		8.3	
Mus musculus	25	3		8.3	
Oryctolagus cuniculus	2,000	60		33.3	
Rattus norvegicus (> 6 weeks old)	200	10		20	
Rattus norvegicus (< 6 weeks old)				10	
Gallus domesticus		64.3	128.5		2

BW : body weight (g)
DFI : daily food intake (g/day)
DWI : daily water intake (mg/l/day)
BW/DFI : conversion factor from mg/kg body weight/day to mg/kg food
DWI/DFI : conversion factor from mg/l/day to mg/kg food

Concentrations causing no effect after long-term exposure (NOEC) are preferred. If, in a study, a single dose or the lowest dose of a range causes < 20 % mortality, a NOEC may be calculated from LOEC/2. If the effect is more than 20 %, the data cannot be used.

Laboratory food for mammals and birds is usually grain. The energy content of grain is higher than fish. This means that in order to obtain the same amount of energy more wet weight of fish must be consumed compared to grain. Therefore a correction factor of 3 may be applied for the difference in caloric content of the diet of laboratory animals and the diet of fish-eating birds or mammals (Everts et al., 1993).

References

Everts JW, Eys Y, Ruys M, Pijnenburg J, Visser H and Luttik R (1993). Biomagnification and environmental quality criteria: a physiological approach. ICES J. Mar. Sci. **50**, 333-335.

Romijn CAFM, Luttik R, Van De Meent D, Slooff W, Canton JH (1993). Presentation of a general algorithm to include effect assessment on secondary poisoning in the derivation of environmental quality criteria. Part 1: Aquatic food chains. Ecotox. Environ. Saf. **26**, 61-85.

Sax NI (1989). Dangerous Properties of Industrial Materials. Sax and Lewis (eds).

Appendix VIII Environmental risk assessment for metals and metal compounds

Introduction

This document gives a general outline on how to perform risk assessments for metals using the methods that are available for risk assessment of new and existing organic chemicals as a starting point. There are a number of fundamental differences between metals and organic chemicals that must be taken into account when assessing the risks to man and the environment, e.g.:

- unlike most organic chemicals, metals, and a limited number of organometallo compounds like methylmercury and methyltin, are a class of chemicals of natural origin. Consequently natural background concentrations and the exposure due to these background concentrations should be taken into account during risk assessment;
- the availability of metals for uptake by organisms under field conditions is limited, will vary from site to site and is highly dependent on the speciation of the metal. Hence, it is of utmost importance that both PEC and PNEC are based on similar levels of availability in both exposure and effect assessment, taking the speciation into account;
- the same toxic form can originate from a variety of different substances, e.g. Zn^{2+} from $ZnSO_4$, $ZnCl_2$ etc. Therefore it is in general necessary to take into account all metal species that are emitted to the environment which in the end lead to concentrations of the toxic form.

Substantial levels of information are available regarding the fate and toxicity of metal ions and this information will be examined to improve the assessment process. However, it is recognised that many of the specific fate and toxicity extrapolations are either not appropriate or need modification. The interaction of metal ions with the media in both the aquatic and soil compartments may result in a high level of uncertainty regarding the true level of bioavailablity of the toxic species necessary for a practical assessment.

Organo-metallic compounds are not explicitly covered by this procedure unless they act, through their degradation products, as significant sources of the toxic metal ion. It is considered that these organo-metallic compounds can generally be assessed as individual substances in accordance with the procedures laid down in the main text (Chapter 3). When the emissions of these substances are major contributors to the toxic metal ion concentration in either a local or regional environment, they will be further assessed according to the procedures laid down in this document.

When describing the topics that need to be taken into consideration for the risk assessment of metals, there is often a misunderstanding with regard to definitions of some of the key terms. In this appendix the following definitions will be used for these key terms:

General

- **total concentration of a metal**: for terrestrial systems, the concentration of a metal that is determined after complete destruction of the mineral matrix. For aqueous systems: the total amount of metal present, including the fraction sorbed to particles and to dissolved organic matter and the fraction in the mineral matrix;
- **available fraction**: the fraction of the metal that is extractable from the substrate with chemical (e.g.: neutral salt, water extraction) or physical means (shaking, pore water

collection), and that is generally considered to be a better estimate for the fraction that is potentially available for organisms than the total concentration;
- **bioavailable fraction**: the fraction that is available for uptake by a specific organism. A single substrate has only one 'availability' for each of the possible physico-chemical extraction procedures. The bioavailability differs, however, per biological species. Thus, taking soil as an example, for instance for worms in a certain soil the bioavailability may be high (it is in this case the concentration in the pore water that determines uptake), while for arthropods in the same soil the bioavailability may be low (uptake by the food is for these organisms the dominant uptake route);
- **natural background concentration**: the concentration that is present due to natural causes only;
- **ambient background concentration**: the concentration that is present due to natural background plus the immission of metals from diffuse sources of human origin[9].

For soils or sediments

- **water extractable fraction or concentration**: the fraction or the concentration of the metal that is extracted after shaking the substrate in aqueous solution (usually distilled water);
- **neutral-salt solution extractable fraction or concentration**: the fraction or the concentration of the metal that is extracted after shaking the substrate in neutral salt solution;
- **pore water concentration**: the concentration of the metal that is present in the pore water collected from the substrate;
- **pore water activity**: the concentration of a metal in the aqueous fraction that is potentially biologically active (usually considered to be the concentration of metal ions that can be taken up by organisms).

Exposure assessment

For the assessment of metals it is in general necessary to take into account all metal species that are emitted to the environment which in the end lead to concentrations of the bioavailable species that may cause effects. In practice, a limited number of major emissions or uses predominate and these must initially be identified. The assessment will normally concentrate on the impact of these emissions since they will be the major contributors to the regional burden, but due care must be paid to the impact of local emissions of specific substances. An inventory of all relevant emission sources must be prepared and specific industry and use categories identified for assessment of both local and regional impact.

Two types of emission can be identified: diffuse emissions and point source emissions. For some metal compounds, diffuse sources such as emissions from agriculture, transport, corrosion etc

[9] In case of soil, for all metals so-called reference lines were derived by correlating measured ambient background concentrations (total concen-trations in the soil-matrix) at a series of remote rural sites in the Netherlands to the percentage lutum (%L) and the organic matter content (%H) of these soils (Ministry of VROM, 1994). The same approach has been followed in Flanders, Belgium (Ontwerp uitvoeringsbesluit, 1995). To this end the 90-percentiles of the ambient background concentrations measured were used. The metal-specific parameters of the regression equations represent the strength of binding of the different metals to soils of different clay and humus contents. The reference lines are not only used to calculate ambient background concentrations at given sites, but also to enable the extrapolation of laboratory toxicity data to standard-soil conditions.
Some typical examples of reference lines derived in The Netherlands ([ ] = ambient background concentration in mg/kg soil, L = % lutum, H = % organic matter): $[Cu] = 15 + 0.6 \cdot (L + H)$; $[Zn] = 50 + 1.5 \cdot (2L + H)$ or $[Ni] = 10 + L$.

can make a significant contribution to the overall levels. For many substances, however, local emissions from point sources will need to be considered as well as the wider contribution to the regional burden. New substances, for example, must be assessed for their impact following local emissions. In general their contribution to the larger environmental burden will be small until high annual tonnages are reached.

Local exposure assessment

As with organic compounds, the precise emissions will need to be identified and quantified for the whole life-cycle of the substance. Emission factors should initially be based on the substance being considered. It is important to know whether the substance is soluble in water, or can be transformed into a soluble form. Thus some knowledge of the chemistry of the particular substance and its interaction with the receiving media is important. Where the metal compound is soluble or can be transformed to a soluble form, the prediction of the environmental concentration, PEClocal, can be based on the relevant soluble metal ion. The behaviour of the substance in a wastewater treatment plant can be modelled using SimpleTreat, although measured Kp values will have to be used (Section 2.3.7 of main text). Since the actual bioavailability of the metal ion will be determined by the properties of the receiving media, such as the pH and water hardness, the precise physico-chemical characteristics of this receiving media must be defined. In general, it will be defined in a way which optimises the bioavailability of the toxic species. Speciation models exist which may be used to determine the soluble fraction. The partitioning behaviour of the substance to sludge/sediment/soil can be based on the appropriate Kp values for the soluble ion.

In some cases, the metal compound will be only poorly soluble and sufficiently stable to not rapidly transform to a water soluble form. In these circumstances, the substance itself should be assessed taking into account its specific partitioning characteristics. For the aquatic environment, it can be assumed as a first estimate that the substance will dissolve up to its water solubility limit, and that this fraction will be the bioavailable form. Refinement of the assessment may take into account kinetics of the dissolution.

Regional exposure assessment

As for organic substances, all emissions from both point and diffuse sources are assumed to contribute to the regional concentration, PECregional. Because of the wide range of transformation processes and longer timescales involved, it is assumed that all the individual metal compounds are changed to the ionic species. Where possible, information on kinetics of transformation processes should be taken into account.

As bioavailability is influenced by various physico-chemical characteristics of the environment it is important to define a 'standard environment', especially for a regional assessment. It is proposed that a regional assessment is carried out under conditions that optimise the bioavailability with respect to ranges for pH, water hardness etc that are found in the natural environment. This environment will probably differ for each metal assessed. Multimedia fate models can be used to assess exposure of man and ecosystems to metals on a regional scale. In applying multimedia fate models all emissions, including point sources, are assumed to be diffuse.

Transport of metals between the aqueous phase and soil/sediment/suspended matter should be described on the basis of measured soil/water, sediment/water and suspended matter/water equilibrium partition coefficients (Kp), instead of using common mathematical relationships based on, for example, octanol-water partition coefficients, as is usually done for organic

chemicals (see Section 2.3.4 of the main text). The same applies to the bioconcentration factors required: only experimentally determined values should be used (see Section 3.8 of the main text and Section 3.3 of this appendix). For soils, the Kp values to be used should, as far as possible, be derived for the soil type of interest. The soil usage should also be taken into account (for instance cultivated versus non-cultivated soils) since this may be of importance for the most appropriate Kp values. Often volatilisation is to be ignored. In such cases, most of the metal present in the atmosphere is predominantly bound to aerosols which means that rates of dry and wet deposition (in combination with the scavenging ratio) of atmospheric aerosols will suffice to quantify transport from the atmosphere. If biotransformation occurs this must be taken into account.

More specific guidance on the use of regional fate models is given in **Figure 1**.

In general, the mathematical descriptions of fate processes used in multimedia fate models are also applicable to local models.

Background concentrations

When assessing the exposure of man and ecosystems to metals previous releases into the environment need to be considered. In view of differences in bioavailability (see below) it is important to distinguish between ambient background concentrations and natural background concentrations. One should be aware that natural background concentrations within an environmental compartment may vary from site to site by several orders of magnitude. Also, due to natural dynamic processes like weathering, natural background concentrations may change over time. This means that it is impossible to attribute single values to natural background concentrations of specific metals within a certain compartment. It should be noted that under natural conditions in certain regions, clearly elevated natural background concentrations can be encountered. When assessing the natural background concentration within a certain area, these "outliers" should not be used or included in the calculation of the standard background concentrations as they would give a non-representative picture thereof.

Several methods are available for determining background concentrations. Apart from the obvious method of measuring metal levels at selected sites considered to be undisturbed by human activities, additional methods include:

Geochemical modelling: estimation methods on the basis of the contribution of weathering processes (erosion). This method is shown to be well applicable for assessing natural background concentration in aqueous systems (rivers).

Assessment of metal concentrations in the deeper sediment layers, taking into account anthropogenic contributions and leaching to these layers.

For surface water having ground water as its origin: assessment of the metal concentrations in the deeper ground water.

For soils, ambient background concentrations can be calculated as described above (reference lines). Through this procedure the natural binding capacity of soils, making the metal more or less inert in the solid phase, is approximated. Application of this procedure to both laboratory toxicity data and to field soils is possible.

For surface water extensive national monitoring programs exist for the follow-up of metals in the aquatic environment since most metals are considered in the EC Regulation 76/464 as list I ("black list") or list II ("grey list") substances. Extraction of representative natural background

concentrations may be possible from these data. However, these monitoring programs often measure total instead of dissolved metal concentrations.

Equilibrium partitioning/bioavailability

One should be aware that Kp values are both environment (site) and compound specific, and depend on the speciation of the metal in both the solid and the liquid (pore water) phase. The speciation of metals is strongly influenced by environmental factors like for instance temperature, redox conditions, pH, and composition of both the liquid and solid phase.

Multimedia fate models can be used to estimate exposure to metals. However, there are several differences compared to the use of these models for organic compounds. Below, differences are described for applying regional models. Reference is made to the sections in the main text.

1. Physico-chemical properties (section 2.3.2)

In general water solubility, boiling point and vapour pressure cannot be used. The octanol-water partitioning coefficient is not appropriate and measured partition coefficients K_p should be used instead.

2. Partition coefficients (section 2.3.5)

Adsorption to aerosol particles

Most of the metal present in the atmosphere will be bound to aerosols. Therefore, an extremely low value for the vapour pressure should be used in formula 5 on page 31, e.g. 10-20 Pa. This leads to a value for $Fass_{aer}$ almost equal to one. If a valid measured value is available, this value can be used.

Volatilisation

Volatilisation can be ignored for metals, except for mercury-compounds and several organometallo compounds. Therefore the Henry-coefficient should be set to a very low value (formula 6).

Adsorption/desorption

Formula 8 and 9 cannot be used. As stated in this appendix, measured K_p values must be used for water-soil, water-sediment and water-suspended matter.

3. Biotic and abiotic degradation rates (Section 2.3.6)

Not important for regional models.

4. Elimation processes prior to the release in the environment (Section 2.3.7)

For applying models like SimpleTreat a partition coefficient is used for water-sludge. For metals a measured K_p value must be used. However, it should be noted that K_p values are different for the different metal species.

5. Calculation of $PEC_{regional}$ (Section 2.3.8.7)

The values applied for model parameters for the regional model (Table 10), intermedia mass transfer coefficients (Table 11) and model parameters for the continental concentration (Table 12) can be used.

Figure 1: Use of multimedia fate models for metals

In a natural soil or sediment system, metals can be distributed over the following fractions:

- dissolved in the pore water,
- reversibly or irreversibly bound to soil or sediment particles,
- reversibly or irreversibly bound to organic ligands,
- encapsuled in secondary clay minerals and metal(hydr)oxides,
- encapsuled in the primary minerals.

It is recognised that for various organisms, only the metal species present in the aqueous phase (pore water) are potentially available for direct uptake by biota and thus mainly responsible for effects on biota. Other uptake routes may also be important, especially for metals with high Kp values, but at the moment little is known on how to treat these processes quantitatively in the risk assessment. Processes determining the availability of metals for direct uptake by biota from the aqueous phase include precipitation, dissolution, adsorption, desorption and complexation. All processes mentioned are not only pH-dependent (adsorption of metal cations for instance increases with pH), but are also strongly influenced by competition for adsorption sites and to all complexation reactions likely to increase the solubility of the metal.

At the moment most Kp values are expressed in terms of total concentrations present in both the aqueous and the solid phase. As can be derived from the possible distribution sites for metals mentioned above, availability of metals for uptake by biota can differ from site to site and, due to amongst others weathering and (de)sorption processes, may change over time. At this stage it is of importance to realise that in general the bioavailability of metals in test systems (expressed as the fraction of the total amount of metal present in the system) may be higher than the bioavailability under field conditions.

When performing risk assessment it is of utmost importance that both PEC and PNEC are based on similar levels of availability. What is required is that for both exposure and effect assessment, Kp values are expressed in terms of concentrations available for uptake by biota in both the aqueous and the solid phase:

$$K_p = \frac{\textit{total available concentration in solid phase}}{\textit{concentration in aqueous phase}} \qquad (1)$$

It is of importance to be aware that equation 1 differs from the commonly used expressions for Kp in the sense that instead of total concentrations in both the solid and liquid phase, available concentrations are to be used. Reason for this is that part of the metal present in the solid phase may be incorporated in the mineral fraction and is therefore not available. Several experimental extraction techniques have been developed to determine available concentrations of metals, thus enabling the calculation of Kp values according to equation (1). However, up till now the underlying concepts for a standardised approach towards partition coefficients representing availability have not yet been sufficiently worked out.

Finally, with regard to availability of metals it should be noted that apart from the general processes denoted above, under certain environmental conditions additional complexation and precipitation processes may take place that may strongly diminish aqueous metal concentrations. An example of such a process is the formation of insoluble metalsulphides under anaerobic conditions (the so-called Acid Volatile Sulphide, or AVS-concept).

Monitoring data

Metals are a group of compounds for which relatively many reliable monitoring data in all environmental compartments are present. Given the fact that the group of metals is limited to a small number of compounds, for which usually sufficient monitoring data are available, risk assessment may well be based on monitoring data. In general monitoring data are preferred over model calculations. When interpreting the data, natural background concentrations, ambient background concentrations and availability for uptake by biota need to be taken into account.

One should be aware that for the aquatic environment metal concentrations may sometimes be reported as dissolved concentrations and sometimes as total concentrations. Dissolved concentrations can be derived from total concentrations by means of the concentrations of dissolved organic matter and suspended particulate matter and partition coefficients between water and either organic or particulate matter. Since, as indicated before, risk assessment is to be performed on the basis of availability, dissolved concentrations should preferably be used since these indicate the bioavailable metal fraction in the aquatic environment.

For soils and sediments sufficient information is only rarely available from monitoring data to directly determine the bioavailable metal fraction. By applying the appropriate Kp values, estimates of the available metal concentrations can be obtained. PECs from calculations and PECs from monitoring data can be compared. In cases where calculated PECs are below PECs based on measured concentrations, natural background and ambient background concentrations should be taken into consideration.

Effects assessment

Availability of data

Toxicity data are available for most metals in sufficient quantity, since there are few compounds, and various toxicity data exist at least for the soluble metal salts. Most data are available for the toxic effects of metals on aquatic organisms, to a lesser extent data are present for terrestrial and sediment-dwelling organisms. Usually most data are based on total concentrations of the metals under investigation. For essential metals deficiency data must be taken into account.

The data are available both on short and long-term tests, and are present for species from various trophic levels. These data can be used for the effect assessment in all compartments following the procedures for assessing the adequacy of data as presented in the main text (see Section 3.2). However, some metal-specific criteria must be taken into account:

physico-chemical test conditions that define the metal speciation and bioavailability should be relevant for field conditions: water hardness, pH, alkalinity, presence of complexing agents (humic acids and EDTA);

content of metal already present in the test medium, especially for soils taken from the field and natural waters. As metals are natural constituents of the biosphere these background concentrations can influence the test results. However, it should be noted that the bioavailability of the background concentration for soils is probably less than that of the “added” metal;

for essential metals organisms of a given habitat are conditioned to the natural concentration range for essential elements. Within this range they can regulate their metal uptake in such a way that their internal concentration is kept relatively stable (homeostasis). This implies that organisms tested should originate and be cultivated within this optimal concentration range.

Derivation of the PNEC

PNECs can be derived through the application of assessment factors on the basis of the available data assessed according to the criteria given above. Standard methods applied elsewhere (e.g. for organic compounds) can be used for this (see Sections 3.3/3.7 of the main text). However, because of the specific mode of action that metals may have for some species, care should be taken in extrapolating short-term toxicity data to the PNEC using the standard assessment factors in Section 3.3. For many metals sufficient long-term toxicity data for aquatic organisms may be present to enable statistical extrapolation, results of which can support the results of PNECs calculated using assessment factors.

Calculated PNECs derived for essential metals may not be lower than natural background concentrations.

A prerequisite for the derivation of the PNEC is that it is done on the basis of the same level of availability as in exposure assessment:

Results from aquatic toxicity tests are usually expressed as total concentrations. As a first approach total concentrations have to be recalculated to dissolved concentrations using partition coefficients. If this is not possible, the total concentration can be set equal to the dissolved concentration. Differences in test systems, e.g. (semi-)static versus continuous flow systems and natural versus standard water, have to be considered;

For the terrestrial compartment many data exist, but most are only expressed as total concentration that has been added to the test media. This added amount will be partitioned among the aqueous and the solid phase. Application of partition coefficients to calculate the available concentration in soil can be applied. Soil type correction, using reference lines should be applied to correct for differences among soil types (see also Section 3.6.2 of the main text).

In future risk assessment for the terrestrial compartment one should be aware of the different routes of exposure that exist among terrestrial species: for species that are not exposed through the aqueous phase, the (physico-chemically) available fraction needs not be correlated to the bioavailability;

Some of the metals are essential metals, having a function in biological processes at low concentrations. Shortage of micronutrients may cause malfunction. This implies that in setting the PNEC information on deficiency levels should be taken into account. It should, however, be noted that often no information on deficiency levels of various metals for various species is available.

Though some exceptions exist, in general ionic metal species are considered to be the dominant metal species taken up, and are thus considered to be the metal species responsible for the toxic effect. Data on the concentration of ionic species in aquatic and terrestrial systems are not readily available, and cannot, as yet, be applied on a regular basis in risk assessment.

Bioaccumulation of essential metals

Metals are taken up by organisms. For essential metals, biota regulate their uptake by means of the general physiological mechanism of homeostasis. By this mechanism, organisms will keep within a certain range of varying external concentrations, their intracellular levels relatively constant, in order to satisfy their requirements for that essential element. Homeostasis implies that organisms can deliberately concentrate essential elements if concentrations in the environment are very low. This may lead to high BCF values. On the other hand, the

homeostatic regulation capacity will be exceeded at a given higher external concentration beyond which the element will accumulate and become toxic.

Risk Characterisation

The risk characterisation of metals basically follows the principles set out in Section 4 of the main text. However, it should be stated again that is very important that both PEC and PNEC are based on similar levels of availability. In addition, when PEC/PNEC ratios greater than one are found, it is very important to have information on the natural and/or ambient background levels in order to decide upon further actions to be taken to reduce the risks.

Since for most metals sufficient monitoring data are obtainable, risk assessment will often be based on measured instead of calculated environmental concentrations, especially for a regional assessment. Usually most monitoring data deal with total concentrations. Especially in case of aqueous systems it often is well possible to convert measured total concentrations to dissolved concentrations. For terrestrial systems this is possible by applying the appropriate Kp values.

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Appendix IX Environmental risk assessment for petroleum substances

Introduction

In the present appendix the Hydrocarbon Block Method (HBM) is described, which is under development and may be used for environmental risk assessment of petroleum substances. The method was originally devised by CONCAWE (The Oil Companies' European Organisation for Environmental and Health Protection) and was discussed in a workshop in Ispra in December 1994 (CONCAWE, 1995; EU, 1995). The approach has only recently been devised and hence experience with its application is limited. Although there has been work to validate the general approach, it should be recognised that there are still uncertainties regarding some technical details which should be borne in mind, when considering the outcome of the risk characterisation.

Outline of the method

There are many petroleum substances (e.g. refinery streams and solvents) which although described by a single EINECS number are hydrocarbon mixtures of varying degrees of complexity. The compositional complexity of many petroleum hydrocarbon substances is compounded by the fact that their composition will vary depending on the source of crude oil and the details of the process used in their production. This compositional complexity poses particular problems when environmental risk assessment is required.

Difficulties in carrying out a risk assessment for petroleum substances arise because individual components of them have specific and different physico-chemical and ecotoxicological properties, and potentials to be degraded in the environment. Each will be subjected to different distribution and fate processes on release. This means that on release to the environment, each component will behave independently and reach its own concentration in each environmental compartment. It follows from this, that a PEC for the whole petroleum substance does not exist. It would in theory, be possible to identify each individual component of a petroleum substance and then to determine a PEC for each of them. In practice this approach demands a degree of analytical resolution that is not achievable for most petroleum substances and even where possible, handling such large quantities of data would be impractical. However, since hydrocarbons of similar structure will have similar physico-chemical properties and potentials to be degraded in the environment they will have similar distributions and fates within a given environment. It is therefore possible to group or “block” such hydrocarbons, so that components having similar properties may be considered together (it should be recognised that a “block” may consist of a single component or a large number of components with similar fate and distribution properties). Once the “blocks” for a substance have been established, PEC values can be calculated for each “block” for each environmental compartment. Given that PECs can only be obtained for single components , or groups of similar components, it follows that PNECs must also be estimated for the same individual components or groups of components.

Therefore, ecotoxicity data obtained on the whole substance, whether obtained using water accommodated fractions (WAFs) or dispersions, cannot be used to estimate PNECs. PNECs must be based on the toxicity of the individual “blocks”, be they single or multiple component “blocks”. These blocks should show similar modes of action.

From the above it is clear that the PEC/PNEC ratio of the whole substance cannot be derived directly, as neither the PEC, nor the PNEC for the whole substance will be available. The PEC/PNEC ratio is therefore derived from the PEC/PNEC ratios of the “blocks” of components,

based on the proportional contribution of each of the "blocks" to the composition of the whole substance, and assuming that effects will be concentration additive:

$$\frac{PEC}{PNEC}\ whole\ substance\ =\ \frac{PEC_A}{PNEC_A}\ +\ \frac{PEC_B}{PNEC_B}\ +\ \frac{PEC_C}{PNEC_C}\ etc. \qquad (2)$$

where:
A,B,C etc. are the "blocks".

This is referred to as the Hydrocarbon Block Method (HBM).

In relation to the above it should be noted that where the petroleum substance is of such limited complexity that it can be considered to constitute a single "blocks" (e.g. some narrow-cut hydrocarbon solvents) then the risk assessment is identical to that for a simple single component substance i.e. the substance is a single "blocks" and therefore, the PEC for the petroleum substance and the "blocks" are the same, the ecotoxicity data used to obtain the PNEC can be based on the toxicity of the whole substance, and the PEC/PNEC ratio can be obtained directly.

Given the complexity of many of the petroleum substances and hence the number of "blocks" that will be created, allied with the need for flexibility in the assessment procedures, it is considered that the use of this method of risk assessment for petroleum substances will, in practice, only be possible using computer based assessment procedures.

In view of the fact that particular "blocks" of hydrocarbons may be present in more then one petroleum substance, there may be a need to consider the contribution to the overall environmental risk from more then one petroleum substance. In principle the HBM allows for calculating the combined environmental risks of different petroleum substances in specific situations or for the comparison of combined PEC values with monitoring data. For this, the PEC/PNECs of the different discharged petroleum substances (or the values for their specific blocks) can be combined in the same way as the blocks for a specific petroleum substance are combined, assuming that the effects will be concentration additive.

Outline of the application of the hydrocarbon block method

The following outlines the principal steps in the application of the HBM:

- obtain compositional data for the substance that are sufficient to assign components to "blocks";
- define "blocks" by grouping components on the basis of similar structural and/or physico-chemical properties, degradation parameters and ecotoxicological properties. If desired, "blocks"can be defined as single components;
- obtain production and use data;
- establish release estimates for each "blocks". A single release estimate for a petroleum substance may not always be adequate: "blocks" with markedly different physico-chemical properties may require different release estimates;
- assign representative values for physico-chemical properties, degradation rate constants and LC/EC50s and NOECs for each "blocks";
- determine the PEC value for each compartment for each "blocks" (local as well as regional);
- determine the PNEC value for each "blocks"
- calculate PEC/PNEC ratio for each "blocks"and sum proportionally.

Summarising, once the "blocks" with their physico-chemical and ecotoxicological properties are defined, there is no difference between the approach presented in the main text of the Technical Guidance Document and the HBM. This means that a PEClocal and PECregional can be calculated as described in Chapter 2 of the main text and a PNEC can be derived as described in Chapter 3 of the main text.

Points for special consideration when using the HBM for risk assessment

The more detailed description of certain aspects of the application of the HBM which follows, is largely based on the application of the HBM to risk assessment for the aquatic environment. This is because it is considered that given the present state of the development of environmental risk assessment, and of the use of the HBM in particular, the use of this compartment best exemplifies the principles, applicability and the issues associated with the use and further development of the HBM.

Composition of petroleum substances

The composition of many petroleum substances is complex, with a single substance often containing a large number of component chemicals, varying in chemical type, molecular weight and isomeric structure.

For some petroleum substances the differences in the physico-chemical properties of the different "blocks" will be such that a single release estimate for the substance may not be sufficient and separate release estimates for some "blocks" or groups of "blocks" may be required.

The complexity of some petroleum substances is further compounded by the fact that their composition may vary depending on the source of the crude oil from which they are produced and the method of their production. It is therefore necessary, that adequate information be available not only on composition but also, where relevant, on variations in composition. This information can be used to allow several calculations of the PEC/PNEC for a substance to take account of likely variations in composition. For petroleum substances, adequate information on composition may allow risk assessment of groups of substances to be undertaken at the same time, for example whole groups of naphthas or kerosines.

It is clear that for many petroleum substances a complete resolution of the composition is neither achievable nor necessary to be able to carry out a risk assessment. But it is essential that compositional data, including information on variability, is sufficient to allow "blocks" to be properly defined for the purpose of risk assessment.

It should be borne in mind that some petroleum substances will contain a relatively narrow range of components and be much more consistent in composition e.g. some narrow-cut hydrocarbon solvents. In some cases it may be appropriate to regard such substances as a single "block".

Many of the components of petroleum substances will be present in many of the substances. In general it is desirable to ensure, that when similar components are present in different petroleum substances the same approach to "blocking" is taken. This will allow the development of PEC/PNEC ratios for "blocks" applicable to a range of petroleum substances (data on physico-chemical and degradation properties and toxicity values for these "common blocks" will only need to be generated once).

Definition of "blocks"

"Blocks" will primarily be defined on the basis of those physico-chemical and degradation properties that are key in determining the distribution and fate of their components. Care should be taken to ensure that "blocks" are not so wide as to encompass components that will not have broadly similar fates and distributions on release. Similarly, "blocks" should, whenever possible, contain substances with a similar mode of action and a narrow range of toxicity. Both the fate and toxicity criteria for "blocks" definition need to be satisfied simultaneously.

Verburgh et al. (1995) carried out "trial calculations" using the HBM based on data for 500 hydrocarbons with a non-specific mode of action, using non-polar narcotic toxicity QSARs and with the Mackay level III model of the EU standard environment defined for calculating the PECregional. It appeared that for definition of the "blocks" the log Kow is the main parameter. This implies that "blocks" can be defined on equally spaced log Kow values: e.g. <3.0; 3-3.5; 3.5-4.0 etc.

It is proposed to start with such a "block definition" for application of the HBM. Based on the results of the risk assessment the "blocks" may be further refined.

"Blocks" based on, or containing, non-hydrocarbons

Certain petroleum substances contain non-hydrocarbon components. Special care should be taken when assessing these substances to ensure that "blocking" is appropriate and in particular that the range of toxicities of components in the "block" is small and that where necessary, due account is taken of differences in mode of action.

Additivity of toxicity

It is generally accepted that for chemicals with the same mode of action, acute toxicities can be considered as additive (EIFAC, 1987). There is increasing evidence that this is also true for chronic toxicity (Hermens, 1989).

Whether a chemical or a group of related chemicals act by non-polar narcosis can be based on a comparison of test results with QSAR estimates for base-line toxicity. Schemes exist that allow the classification of large numbers of organic chemicals according to their mode of action (Verhaar et al., 1992).

Petroleum hydrocarbons are for the great part composed of hydrocarbons. These act via a similar mode of toxic action, non-polar narcosis. In the light of the above it can be assumed that for the hydrocarbon components of petroleum substances, effects will be simple concentration additive.

The situation is less clear with regard to chemicals with different modes of action. Components of petroleum hydrocarbons with specific modes of action are likely to be "blocked" together, provided they have the same specific mode of action. In the first instance the PEC/PNEC ratio of this "block" shall be added to the total PEC/PNEC ratio. From this it will be clear if the PEC/PNEC ratio for that "block" influences any potential for environmental risk for the specific petroleum substance. If it does, further investigation whether or not there is additivity of the modes of action, would be required.

Chemicals which may have a specific mode of action present in petroleum substances can be metallic constituents (e.g. vanadium and nickel in crude oil, fuel oils and asphalt) and heterocyclic compounds (e.g. carbazole compounds in cracked fuels) and mutagens/ carcinogens (e.g. PAHs such as benzo(a)pyrene, 7,12-dimethylbenzo(a)anthracene. However, they are

present in low concentrations compared to the non-specific acting components. Nevertheless, these specific acting constituents should on a case-by-case basis be taken into account in the environmental risk assessment at least in a qualitative way.

QSARs

The identification of the blocks when applying the HBM may be dependent on the use of QSARs for the estimation of physico-chemical properties (e.g. log Kow, water solubility, melting point and vapour pressure) and degradation rates (e.g. photodegradation and hydrolysis rates), when measured values are not available. There are reasonably well accepted methods for the generation of these data using readily available data bases, or QSARs. There are no widely accepted QSARs for biodegradation, but it is considered adequate, at least for screening, if experimentally determined rate constants for the "blocks" of interest are not available, to use QSAR estimates for block identification, according the principles laid down in Chapter 4 on the Use of QSARs.

The use of QSARs is well established for predicting the acute toxicity of simple hydrocarbons, and can be used to supplement the available ecotoxicity data. Whilst the accuracy of QSARs for more complex hydrocarbons and for chronic toxicity may need further consideration, they provide an adequate default where experimental data are not available (in particular where the values are found not to be key to the outcome of the risk assessment).

The minimum data-set available for each priority petroleum substances, is usually not sufficient for risk assessment using the HBM, because it will usually comprise tests conducted with the whole petroleum substance. Since in the HBM process individual hydrocarbons are blocked together on the basis of their environmental fate and ecotoxicological properties, additional data on these hydrocarbons are also required. These may be measured data, but it is foreseen that values derived from QSARs will be helpful for filling datagaps in the establishment of blocks. When the overall risk assessment for the petroleum substance is undertaken (with the PEC/PNEC ratios for the blocks calculated and summed), those blocks contributing most to the overall PEC/PNEC ratio can be identified. It should be noted that any decision on the final outcome of the risk assessment when the overall PEC/PNEC ratio is close to or greater than one, will need to be based on measured (rather than QSAR) data. Hence, for each block (unless the contribution of the particular block is found to be irrelevant to the outcome of the risk assessment), representative measured base-set data should be available. These data could be on any component of the block, since by definition, blocks are comprised of hydrocarbons with similar fate and ecotoxicological properties. Data on some individual hydrocarbons suitable for this purpose, are already available as the IUCLID database shows.

For "block" identification, QSARs for short (algae, daphnids and fish) and long-term (daphnids and fish) toxicity are given in Chapter 4 on the use of QSARs. These QSARs can be used for chemicals with a non-specific mode of action, i.e. for most petroleum substance components. Considering the assessment factors presented in the TGD (see Section 3.3.1 of the main text) a factor of 10 on the QSAR derived long-term NOEC is proposed. More guidance on the use of QSARs in general can be found in Chapter 4.

"Blocks" which do not exhibit acute toxicity

There will be a number of "blocks" for which no acute toxicity is indicated at the limit of water solubility. Adema (1986, 1991) found no short-term toxicity for n-decane or higher homologues and for alkylbenzenes with a carbon number higher than 14. This does not necessarily mean that

these “blocks” will not contribute to chronic toxic effects. There may be several approaches to estimate chronic toxicity for such chemicals if there are no measured long-term toxicity data available:

- use the QSAR for long-term toxicity as presented in Chapter 4 of the TGD. However, these QSARs can only be applied in a range of log Kow from approximately 2-6. For chemicals with higher log Kow the resulting NOEC is often higher than the water solubility.
- for blocks which do not demonstrate acute toxicity at or below their water solubility, QSARs (irrespective of the fact that the result may exceed the water solubility) may be used as a basis for the PNEC by application of a suitable assessment factor. This calculated value is taken to represent the PNEC of the block unless, it is itself greater than the water solubility. In this case the water solubility should be substituted as the PNEC. It should be noted that for very high log Kow values, this may lead to unrealistic PNEC values;
- as an indication above log Kow 6, a parabolic equation to derive a BCF for fish can be used (see Section 3.8.3.2 of main text and Chapter 4) in combination with the critical body burden concept (McCarty & Mackay, 1982) to calculate the chronic toxicity. This critical body burden concept indicates that the long-term critical body burden is equal to the NOEC multiplied by the BCF (CBB = BCF · NOEC) (Sijm et al., 1992; ECETOC, 1995). To be able to perform a risk assessment, there may be a need to develop measured chronic data to support this QSAR prediction.

Undissolved material

Petroleum substances (or components of them) can enter the aquatic environment either in solution or as undissolved material in slicks or dispersions. Hydrocarbons in undissolved form might have direct local effects. It is considered that undissolved hydrocarbons will not be present at the regional level, but in any event this will have to be confirmed by calculating the PECregional.

Monitoring data

For substances consisting of only a single component sound and relevant monitoring data may be available for several compartments. For petroleum substances there are a number of difficulties related to the use of monitoring data that need specific consideration. Frequently there will be measurements of total hydrocarbons or of particular hydrocarbon components that may have come from a range of different petroleum substances.

Such release or monitoring data may be used to provide a worst-case estimate of the concentration of a “block” for screening purposes, assuming that the whole of the release is attributable to the particular petroleum substance. However, it should be noted that the measured concentrations represent the sum of all sources of a block whereas the calculated concentrations for a specific “block” represents only the fraction of the total concentration of this “block” in the environment related to the specific petroleum substance under study. Therefore, monitoring data are most suitable for the assessment of a certain “block”, as they represent the actual concentration the organisms are exposed to in the environment, related to all relevant sources.

Compartments other than the aquatic

The description of the use of the HBM for the environmental risk assessment of petroleum substances given above, has focused on the aquatic environment. This is because at the present time it is only for this environmental compartment that sufficient data and experience are

available to allow anything approaching a full risk assessment. However, the principles of the HBM are applicable to all environmental compartments and it is anticipated that as familiarity with the approach extends, knowledge will increase and it will prove possible to apply it to the soil and air compartments. Particular shortcomings in relation to its wider application at the present time are the lack of data on the toxicity of chemicals, including hydrocarbons, to terrestrial organisms and hence the absence of adequate (Q)SARs.

Contribution of computer based risk assessment to the use of the HBM

The use of computer based risk assessment provides the capability to carry out many iterations of the risk characterisation which in turn facilitates:

- investigation of effects of compositional changes;
- investigation of alternative "blocking" schemes;
- identification of blocks which are the principal contributors to the PEC/PNEC ratio for the whole substance and therefore, where most refinement of the data, through for example the generation of experimental values as opposed to (Q)SAR estimates would be most valuable;
- maintenance of a data base of information on "blocks" which are common to more than one petroleum substance.

Testing strategies

Based on the identification of the blocks, the estimation of the block properties and the compositional information in combination with exposure scenarios a PEC/PNEC is calculated. If this PEC/PNEC is > 1, the general guidance concerning testing strategy as presented in Section 5 of the main text will be followed. Further refinement of the PEC or PNEC may be necessary in order to improve the data estimates for the properties of the blocks.

A form of "sensitivity analysis" may be useful in confirming the selection of blocks to represent a particular petroleum substance; this approach may also be used to identify those particular parameters which are important in defining the fate and effects of the block. This approach may be useful to identify the most relevant additional data that would influence the outcome of the risk assessment.

Further refinement of the data estimates for the block properties should be made when:

- specific blocks have PEC/PNEC values > 1 or;
- the total sum of the blocks results in a PEC/PNEC ratio > 1.

For the blocks with a PEC/PNEC ratio > 1, one or some representative components should be selected. For these component(s) the testing principles from the TGD can be followed and the results can be used as representative for the specific block. If the combination of blocks with individual PEC/PNECs < 1 gives a PEC/PNEC > 1 it is suggested to focus on the major contributing blocks. For the relevant blocks again representative components can be selected and the general testing principles applied.

Application of the method to other UVCBs

It is apparent that this method may be applicable to other UVCB substances, but this will need to be explored on a case-by-case basis. Its broader applicability will be determined by the ability to define acceptable "blocks" and to provide the necessary data to support the derivation of PECs

and PNECs for the “blocks” and for their additivity, which is needed to be able to derive an overall PEC/PNEC ratio.

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Appendix X Transformation pathways

In the table below biodegradation and transformation pathways of some organic compounds are summarised. The mechanisms and pathways presented here are not comprehensive and other mechanisms and pathways may therefore occur. It should also be noted that the assessment of transformation pathways may be complicated due to the interaction between different functional groups within a molecule. The following references give further detail:

Neilson AH (1994). Organic Chemicals in the Aquatic Environment: Distribution, Persistence, and Toxicity. Lewis Publishers, Boca Raton, FL, USA, 448 pp.

Larson RA and Weber EJ (1994). Reaction Mechanisms in Environmental Organic Chemistry. Lewis Publishers, Boca Raton, FL, USA.

GROUP	METABOLIC PATHWAY	TRANSFORMATION PRODUCT(S)
Aldehydes	Oxidation	Carboxylic acids
Alkanes, branched acids	Oxidation/carboxylation	Alcohols/carboxylic
Alkanes, unbranched	beta-Oxidation	Alcohols, carboxylic
Alkanols	Oxidation	Aldehydes, ketones
Alkenes	Epoxidation	Epoxides, diols
Alkynes	Addition of water	Ketones
Amides and related compounds	Hydrolysis	Amines, carboxylic acids
Amines, primary/secondary/tertiary	Oxidative deaminiation/reductive dealkylation/reductive dealkylation	Carboxylicacids/primary amines/secondary amines
Anilines	Ring oxygenation	Catechols
Aromatic hydrocarbons	Oxygenation	Catechols
Azo compounds, aromatic	Reduction	Anilines
Carbamates	Hydrolysis	Amines, alcohols
Carboxylic acids	beta-Oxidation	Acetic acid
Catechols	Oxidation with ring cleavage	Carboxylic acids
Esters (carboxylic/sulfuric/ phosphoric)	Hydrolysis	Alcohols and carboxylic/ phosphoric/sulfuric acids
Ethers, aliphatics	Reductive or oxidative dealkylation	Alcohols
Halogenated aliphatics	Hydrolysis/elimination/reductive dehalogenation	Alkanols/alkenes/alkanes
Halogenated aromatics	Oxygenation	Halogenated catechols
Heteroaromatics	Oxygenation	Similar to aromatics
Ketones	Monooxygenation	Esters
Nitriles	Hydrolysis	Amides, carboxylic acids
Nitro compounds	Reduction	Amines
Nitro aromatics	Dioxygenation (elim. of NO_2^-)/ reduction	Catechols/anilines
Organomercurials (C-Hg bond)	Reductive cleavage	Alkanes,inorg.mercury
Organophosphonate (C-P bond)	Reductive cleavage	Hydroxybenzoates/catechols
Phenols	Carboxylation (anaerobic)/ Oxygenation (aerobic)	Hydroxybenzoates/catechols
Sulfoxides	Reduction	Thioethers, thiols
Sulphonates, aromatic	Elimin. of sulfite by dioxygenation	Catechols
Sulphates, alkyl	Hydrolysis	Alcohols, inorg. sulphate
Ureas	Hydrolysis	Amines

Appendix XI Environmental risk assessment for ionising substances

Introduction

The degree of ionisation of an organic acid or base greatly affects both the fate and the toxicity of the compound. The water solubility, the adsorption and bioconcentration, as well as the toxicity of the ionised form of a substance may be markedly different from the corresponding neutral molecule.

When the dissociation constant (pKa/pKb) of a substance is known, the percentage of the dissociated and the neutral form of the compound can be determined. For example, for an acid with a pKa of 5.5, the pH dependency of the behaviour of the substance can be described as follows:

- 1% dissociated at pH 3.5;
- 10% dissociated at pH 4.5;
- 50% dissociated at pH 5.5;
- 90% dissociated at pH 6.5;
- 99% dissociated at pH 7.5.

Thus, even slight changes in the pH of the environment considerably affect the form in which the substance is present in the environment. This is the case especially for substances with pKa/pKb values around the pH values of the environment (i.e. pH 4-9 for surface water). In the assessment of ionised substances, due attention has to be paid as to how much fate and effects of the substance are affected by the pH of the environment.

Exposure assessment

The water solubility of organic acids and bases are very much dependent on the pH. The water solubility of the dissociated compound can be orders of magnitude higher than the neutral species. Therefore, the pH dependence of the water solubility should be known. At least the pH of the test water needs to be identified. This also applies to log Kow.

The basic parameters used in the exposure assessment (log Kow, Henry's law constant, adsorption/desorption coefficients) are only applicable to the non-ionised form of the substance. Therefore, every time when partitioning of a substance between water and air or solids is concerned, a correction needs to be made in order to take only the undissociated fraction of the compound into account at a given pH. In practice, this implies that Henry's law constant and Kp in soil, sediment, and suspended solids need to be corrected. This can be done by using the following correction factor:

$$CORR = \frac{1}{1 + 10^{A\,(pH\,-\,pKa)}}$$

where:

A	1 for acids, -1 for bases
pH	pH-value of the environment
pKa	acid/base dissociation constant

The above correction can only be used for partitioning coefficients which refer to the unionised form of the substance. This means that for estimated partitioning coefficients, water solubility

and Kow need to be determined for the neutral form. The choice of relevant pH values to be used in the calculation should be based on the pKa/pKb of the compound in concern and any relevant knowledge of the actual toxic form of the substance. For experimentally determined partition coefficients the need for correction should be assessed on a case by case basis, depending on the pH in the test.

These principles apply also to the fate of the substance in sewage treatment plant. However, since the STP is a well buffered environment, a default pH of 7 can be used in the calculations. The role of pH in the experimental determination of the bioconcentration should also be acknowledged.

Effects assessment

Ionisation can markedly alter the toxicity of the substance. Normally, this is caused by the different bioavailability of the dissociated and neutral species. Consequently, when testing toxicity, the tests should preferably be carried out at both sides of the pKa, to fully characterise the possible differences in toxicity. Since this may not be possible in every case, the role of pH should at least be discussed qualitatively in the assessment.

Risk characterisation

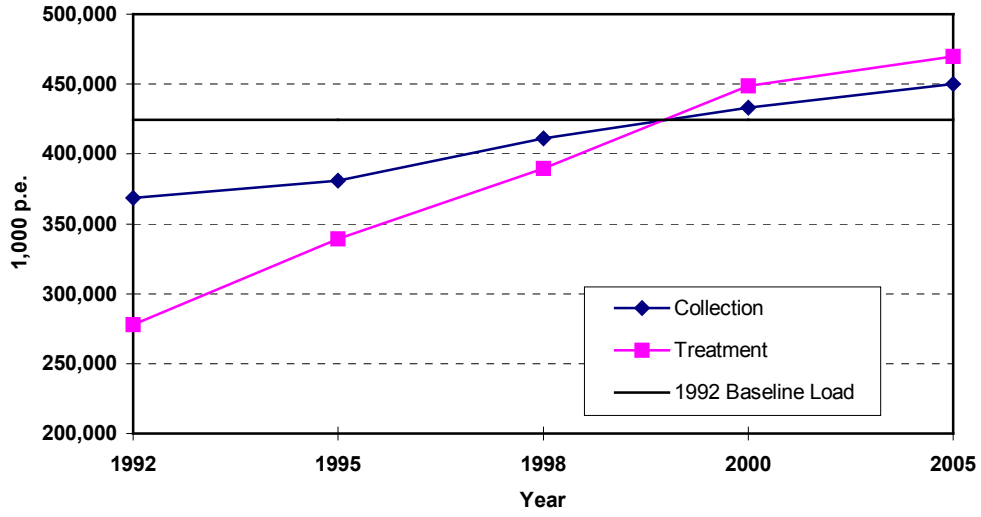
Care should be taken that the PEC and the PNEC in the risk characterisation represent similar conditions. PEC/PNEC comparisons should preferably be made at both sides of the pKa values, within environmentally relevant pH-range. The higher PEC/PNEC ratio should be used in the risk characterisation, following the realistic worst-case approach. If it is not possible to carry out a quantitative analysis, the assessor should take the pH effect into account qualitatively.

Appendix XII Connection to Sweage Treatment Plants in Europe

Default STP Connection Rate

Marked improvements in overall EU wastewater collection (+22% relative to 1992) and treatment (+69% relative to 1992) will follow full implementation of the Urban Waste Water Treatment Directive (91/271/EEC) in 2005 (see Figure 1). Even before 2005, a provisional figure is indicated for interim use as substantial increases in wastewater collection (+12%) and treatment (+40%) capacity have already been reported from across the EU. Projected wastewater treatment capacity in the EU as a whole for 2000 is greater than baseline organic loadings (i.e., 106%), although this is not uniformly distributed throughout the EU. An interim figure of 80% connection to wastewater treatment is therefore proposed for the generic region. A figure of 90 - 95% is also proposed for use following full implementation of the UWWTD. This coincides with the likely ultimate degree of connection and treatment capacity for urban regions of the EU.

Figure 1. - Development in Collection and Treatment Capacity EU14 (Source: EC, 1999)[10].



p.e. = person equivalent

Historical Data

Data on the proportion of the total population connected to wastewater treatment in individual MS in the period 1970-95 are presented in Table 1. The population weighted average for the whole of the EU15 in 1995 was 73%. Although the apparent degree of connection to wastewater treatment is low in some countries, its absence does not necessarily always imply inadequate treatment or direct discharge. For example, the proportion of the population with individual arrangements such as septic tanks has been reported as 24% inGreece, 23% in France, 22% in Finland, 12% in Portugal, 7% in Germany, 6% in Italy, 2.5% in the UK, 1.5% in the Netherlands, 1% in Spain and 0.5% in Luxembourg (EWWG, 1997)

[10] European Commission (1999). Implementation of Council Directive 91/271/EEC of 21 May 1991 concerning urban waste water treatment as amended by Commission Directive 98/15/EC of 27 February 1998. Summary of the measures implemented by the member states and assessment of the information received pursuant to Article 17 and 13 of the directive. Available on European Union (EU) web-site at http://www.europa.eu.int/water/water-urbanwaste/report/report.html.

Table 1 Proportion of the Population served by a Wastewater Treatment Plant (Eurostat/EC/EEA, 1998)

Member State	Year				
	1970	1980	1985	1990	1995
Belgium	4	23	-	-	27
Denmark	54	-	91	98	99
Germany	62 (West)	80 (West)	84 (West)	86	89
Greece	-	1	10	11	34
Spain	-	18	29	48	48
France	19	62	64	68	77
Ireland	-	11	-	44	45
Italy	14	30	-	61	61
Luxembourg	28	81	83	90	88
Netherlands	-	73	87	93	96
Austria	17	38	65	72	76
Portugal	-	2	4	21	21
Finland	16	65	72	76	77
Sweden	63	82	94	94	95
UK	-	82	83	87	86

Urban Waste Water Treatment

Details of the current situation within the EU reveal that there are 17,351 agglomerations of more than 2,000 p.e. in the 14 member states excluding Italy (EC, 1999). This represents a total organic loading of 424 million p.e. relative to an actual EU14 population of 314 million. Data from a different source indicate an organic load of 105 million p.e. (in Italy (EEWG, 1997)).

It is notable that relatively few countries (i.e., Greece, Spain, Portugal and the UK) have designated coastal/estuarine areas as less sensitive. Discharges to such areas are subject to less stringent requirements regarding treatment (i.e., primary). In p.e. terms, this corresponds to <9% of organic loads.

Details of developments in the capacity of collecting systems conforming to the provisions of the directive are presented in Figure 1. The projected increase in capacity in terms of absolute p.e. (81 million) and percent (+22%) between the baseline situation in 1992 and the final situation after implementation of the directive in 2005 is substantial. More marked increases are projected for individual MS such as Spain (+113%), Ireland (+346%) and Portugal (+76%). Separate data for Italy indicate an increase in collection capacity of 7% from a baseline of 95 million p.e. to 102 million p.e. in 2005 (EEWG, 1997).

Details of developments in treatment capacity conforming to the provisions of the directive are also presented in Figure 1. Increases up to 1998 and those further forecast up to 2005 are significant in most MS except Finland, the Netherlands and Sweden where existing capacity was high. Projected overall increases for individual MS include +320% for Greece, +209% for Spain, +689% for Ireland and +186% for Portugal. The overall increase in capacity forecast for the combined EU14 (excluding Italy) at the implementation deadline (2005) is 191 million p.e. or +68% compared to 1992 baseline capacity. Reported increases up to 1998 are 112 million p.e. or

+40% compared to 1992. Increases to date in individual member states include +27% for Germany, +51% for France, +82% UK, +91% for Spain and +95% for Portugal. It has been concluded that by the implementation deadline, the capacity of the treatment plants would be sufficient to treat the total projected combined organic load for agglomerations >2000 pe in all the 14 EU MS (EC, 1999). Indeed, projected final treatment capacity (469 million p.e.) is approximately 11% greater than the total organic load (424 million p.e.). However, distribution of treatment capacity will not necessarily be homogenous. For example, projected treatment capacity post-implementation exceeds 1992 baseline organic loads by +28% in the Netherlands, +35% in Germany and +74% in Sweden. Treatment capacity in Italy is forecast to increase by 73% from a baseline of 59 million p.e. to 102 million p.e. in 2005 (EEWG, 1997).

Appendix XIII Risk assessment of sources not covered by the life-cycle of the substance

Introduction

Exposure may occur from other sources than the life-cycle of the produced or imported substance under assessment. Such sources have been referred to as "unintentional sources". Examples are substances of natural origin, substances formed in combustion processes and indirect emissions of the substance, e.g. as by-product, contaminant or degradation product of another substance. In these cases information is necessary on emissions which are not covered by the life-cycle of the substance being assessed.

Knowledge of the extent of the sources not covered by the life-cycle of the substance under review is necessary for a full evaluation of the risks posed by the priority existing substance or biocidal product. The information is needed for example for a correct interpretation of measured environmental concentrations. The information is also required for an evaluation of the relative contribution of the emissions of the substance under review to the overall risks posed by the substance through all possible sources. Such information might be relevant in the eventual development of a risk reduction strategy.

In this appendix some recommendations are given on how to deal with these kind of sources, based on the practical experience gained with the implementation of the ESR. There is still a need for an EU decision on how to handle these cases at the time of revision of the TGD.

Legal background

The Existing Substances Regulation (EEC) 793/93 (ESR) requires that all information needed to carry out the risk assessment of a priority substances is submitted to the rapporteur by the Producers and Importers of the substance. The risk assessment however is one of a selected priority substance, the sources of which can be from the produced and imported substance, but also from other sources. Commission Regulation (EC) 1488/94 for example foresees that the risk assessment of a priority substance entails an exposure assessment which, in particular is to consider the exposures resulting from the life-cycle of the produced and imported priority substance, but need not do so exclusively. The Biocidal Products Directive (98/8/EC) (BPD) states that cumulation of effects from the biocidal products containing the same active substances shall be taken into account, where relevant, in the assessment of a biocidal active substance.

Recommendation for sources not covered by the life-cycle of the substance

The rapporteur should clearly list other sources, which can give rise to exposure by the substance being assessed. The risk assessment should include as much readily available information on these sources as possible. Whether or not this information can be taken into account in the risk characterisation is dependent on the quantity and quality of the available information. If there is not sufficient confidence in the available database to make a conclusion of concern/no concern, the risk assessment should be finalised with the conclusion "further information is needed" (Conclusion (i)).

If the emissions originate from the life-cycle of another substance that can be prioritised under the ESR (i.e. a substance listed in EINECS), it is *not required* to take these sources into account in the risk characterisation, as they can be covered by prioritising the other substance. If the

other substance is being assessed, then the risk assessment of the original substance *must* be taken into account in the risk assessment of the other substance.

If the emissions can not be covered by the ESR or BPD, the rapporteur is recommended to use the available information on these emissions as far as possible to carry out a risk characterisation. In the case that "further information is needed" (Conclusion (i)), then, in general, it can not be the obligation of the producers or importers of the substance under examination to obtain such information.

For biocides, sources which include substances of natural origin or releases from other biocidal uses should be taken into account in the risk assessment. When it comes to cumulative effects of a substance used also outside the scope of the BPD (e.g. in plant protection products) and maybe regulated with another Directive there is, at the time of revision of the TGD, still a need for a common EU decision on how to handle such cases. Exclusion of other than only biocidal uses from the assessment causes difficulties, for example, when using monitoring data or comparing measured residue data with Maximum Residue Limits.

Appendix XIV Information on the difference in diversity between saltwater and freshwater

The greater diversity of species in saltwaters[11] compared to freshwaters has been recognised for many years. In the key work "The Seas", Russell and Yonge (1928) state that "The sea is far richer in different forms of life than the land or freshwater, many groups of animals being exclusively marine". This view has been consolidated in other publications which have based the difference on a number of factors including the fact that life originated in the seas and they have been well populated since the earliest fossil records (Tait, 1978).

The results below show recent comparative data on freshwater and saltwater species diversity generated for the Danish Environmental Protection Agency by the Zoological Museum and the Department of Evolutionary Biology at University of Copenhagen.

Taxonomic group	No. of species	Comments
Porifera	4,850	(150 in freshwater)
Ctenophora	50	(Exclusively marine)
Cnidaria	7,000	(Exclusively marine)
Tubellaria	2000	(1000 in freshwater)
Trematoda	6,000 (internal parasites)	------
Cestoda	3,500 (internal parasites)	------
Nemateans	900	(Predominantly marine)
Gastrotricha	150	(Marine and fresh water)
Nematoda	5,000	(15,000 described species in total including parasites and terrestrial, marine and freshwater forms)
Nematomorpha	4	(316 in freshwater)
Achantocephala	1,150 (internal parasites)	-----
Kinorhyncha	150	(Exclusively marine)
Priapulida	17	(Exclusively marine)
Loricifera	100	(Exclusively marine)
Gnatostomolida	80	(Exclusively marine)
Rotifera	100	(1,400 in freshwater)
Polychata	5-10,000	(1000 in freshwater)
Oligochaeta	------	(Many species; mainly in freshwater)
Echinodermata	7,000	(Exclusively marine)
Brachiopoda	300	(Exclusively marine)
Echiura	140	(Exclusively marine)
Sipunculida	350	(Exclusively marine)
Pogonophora	120	(Exclusively marine)
Tardigrada		(Taxonomic group discovered a few

[11] Except those where there are extremes of environmental conditions

Taxonomic group	No. of species	Comments
		decades ago. A few hundred species known from both terrestrial, fresh- and marine water)
Arthropoda		
Chelicerata		
Merostomata	4	(Exclusively marine)
Pygnogonida	1,000	(Exclusively marine)
Insecta	400	(25-30000 in freshwater)
Crustacea		(5-6000 in freshwater)
Entomostraca	10,100	(3000 in freshwater)
Malacostraca	19,000	(3000 in freshwater)
Mollusca		
Gastropoda	19,000	(4000 in freshwater)
Bivalvia	5,450	(2,550 in freshwater)
Scaphopoda	350	(Exclusively marine)
Cephalopoda	600	(Exclusively marine)
Bryozoa	5,000	(70 in freshwater)
Hemichordata	100	(Exclusively marine)
Chordata		
Tunicata	1,300	(Exclusively marine)
Cephalocordata	25	(Exclusively marine)
Vertebrata		
Pisces	15,000	(Guestimate but believed to be an underestimate number of freshwater species less than number of marine species)
Amphibians		(Mainly freshwater)
Mammals	60	(Guestimate)

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European Chemicals Bureau (ECB)

Technical Guidance Document on Risk Assessment
in support of

Commission Directive 93/67/EEC on Risk Assessment
for new notified substances

Commission Regulation (EC) No 1488/94 on Risk Assessment
for existing substances

Directive 98/8/EC of the European Parliament and of the Council
concerning the placing of biocidal products on the market

Part II

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