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SUPERSEDED GUIDANCE - NEWER VERSION AVAILABLE

Guidance on the Biocidal Products Regulation

Volume IV Environment - Part B Risk Assessment (active substances)

Version 1.0
April 2015

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European Chemicals Agency

Mailing address: P.O. Box 400, FI-00121 Helsinki, Finland
Visiting address: Annankatu 18, Helsinki, Finland

DOCUMENT HISTORY

Version	Changes
Version 1.0	First edition (active substances only)

PREFACE

This document describes the requirements under the BPR with regard to effect/hazard-, exposure- and risk assessment for a biocidal active substance. It represents Volume IV, Part B in the new guidance structure. This version (v1.0) only contains guidance for active substances; guidance for biocidal products will be added in a future update, which may take the form of a separate document.

The basis of this document is the EU-TGD of 2003, which was adapted with regard to references and content of the BPR. In addition any text from existing other guidance under the BPD was merged in case it was not covered by the TGD (e.g. text from e.g. the TNsG on BPR Annex I inclusion and TNsG on product evaluation but also existing specific guidance on e.g. rapidly degrading substances). This was done in order to concentrate environmental risk assessment related text in only one single document to have one common basis for future revisions.

The numbering of chapters, tables and equations was kept as far as possible as in the TGD of 2003. However, the chapter of marine risk assessment was split and distributed to the main chapters Exposure and effect assessment which triggers that the numbering of tables and equations changes starting with chapter 3.9.

The former Appendix I of the TGD (containing emission factors for the tonnage-based approach for emission estimation including the A and B tables) was changed to Appendix 7 to this Part B.

The former Appendix II of the TGD (containing tables to estimate the distribution in the STP) was not taken over since the distribution in the STP should be calculated with EUSES or Simple Treat (decision of TM I 2011) because the calculations are more accurate.

New developments in the exposure, effect and risk assessment described in the Manual of Technical Agreements (MOTA), version 6 and the Evaluation Manual (prepared by NL) were included in this document mainly in the form of “Infoboxes”. The MOTA will continue to exist (as TAB: Technical agreements for Biocides) and those parts of MOTA v.6 that did not fit-in to the guidance have been carried forward to the TAB, prepared by ECHA.

NOTE to the reader:
This document is foreseen to begin a first update later this year (2015) to address issues flagged by the BPR Working Group on Environment. At the same time references and minor formatting/editing issues will also be addressed.

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List of Abbreviations

Standard term / Abbreviation	Explanation
AA-EQS	Annual average water quality standards
ACR	Acute to chronic ratio
AOPWIN	EPI Suite software to estimate the atmospheric oxidation rates (US EPA)
AVS (-concept)	Acid Volatile Sulphide
BCF	Bioconcentration factor
BMF	Biomagnification factor
BPD	Directive 98/8/EC of the European Parliament and of the Council of 16 February 1998 concerning the placing of biocidal products on the market
BW	Body weight (g)
BW/DFI	Conversion factor from mg/kg body weight/day to mg/kg food
CAR	Competent Authority report
CBB	Critical body burden
CLASSIC	Community Level Aquatic System Studies Interpretation Criteria (PPP)
CLP	Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006
CONCAWE	The Oil Companies' European Organisation for Environmental and Health Protection
DFI	Daily food intake (g/day)
DRANC	Dutch Risk Assessment System for New Chemicals
DT50	Period required for 50% degradation (define method of estimation)
DWI	Daily water intake (mg/l/day)
DWI/DFI	Conversion factor from mg/l/day to mg/kg food
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
EDTA	Ethylenediaminetetraacetic acid
EEA	European Economic Area
EF	Emission factor
EFSA	European Food Safety Agency
EIFAC	European Inland Fisheries Advisory Commission
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINK	Linking aquatic exposure and effects in the registration procedure of plant protection products

Standard term / Abbreviation	Explanation
EPA (DK, US)	Environmental Protection Agency (of Denmark, or the United States of America)
E-PRTR	European Pollutant Release and Transfer Register
EQS	Environmental Quality Standard
ERC	Ecotoxicologically relevant concentration (ERC)
ETO	Ecological threshold option
EU	European Union
EUBEES	"Gathering, review and development of environmental emission scenarios for biocides" (EU project)
EUSES	European Union System for the Evaluation of Substances
FAO	Food and Agriculture Organization
FOCUS	Forum for the Coordination of Pesticide Fate Models and their Use (European pesticide project for risk assessment)
HARAP	Higher-Tier Aquatic Risk Assessment for Pesticides
HBM	Hydrocarbon Block Method
HEDSET	Harmonised Electronic Data Set (EC/OECD)
HELCOM	The Baltic Marine Environment Protection Commission
HPVC	High production volume chemicals
IC	Industrial category
UC	Use Category
IFEN	Institut Français de l'Environnement
ISO/DIN	International Standards Organisation/ German Institute for Standardization
IUCLID	International Uniform Chemical Information Database
JRC	Joint Research Centre
KOC	Organic carbon adsorption coefficient
KOM	Partition coefficient normalized to organic matter (L/kg)
KOW	Octanol-water partition coefficient
KP	Solid-water partitioning coefficient of suspended matter
L€CX	Lethal (effective) concentration at a specific mortality rate (X %)
LEMTOX	Ecological models in support of regulatory risk assessments of pesticides Developing a Strategy for the Future
LOD	Limit of quantification
LOEC	Lowest observed effect concentration
LOQ	Limit of quantification

Standard term / Abbreviation	Explanation
MAMPEC	Marine antifoulant model to predict environmental concentrations
MATC	Maximal acceptable toxicant concentration
MC	Main Category
MDD	Minimal detectable difference
MITI	Ministry of International Trade and Industry (Japan)
MOTA	Manual of Technical Agreements of the Biocides Technical Meeting
MS	Member State
NOAEL	No observed adverse effect level
NOEAEC	No observed ecologically adverse effect concentration
NOEC	No observed effect concentration
NTA	Non-target arthropods
OECD	Organisation for Economic Cooperation and Development
OPPTS	Office of Prevention, Pesticides, and Toxic Substances (U.S.-EPA)
OPS	Operational Priority Substances (model)
OSPAR	Oslo and Paris Conventions
PBT/vPvB	Persistent Bioaccumulative and Toxic/ very Persistent very Bioaccumulative
PEC	predicted environmental concentration
pH	pH-value, negative decadic logarithm of the hydrogen ion concentration
PNEC	Predicted no effect concentration
POP	Persistent organic pollutant
PPP	Plant Protection Products
PRISEC	PRIority Setting system for Existing Chemicals
PT	Product-type
QSAR	Quantitative structure-activity relationship
RAC	Regulatory acceptable concentrations
RBT	Ready biodegradability test
REACH	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC
RIVM	Rijksinstituut voor Volksgezondheid en Milieuhygiëne (Dutch National Institute of Public Health and Environmental Protection)

Standard term / Abbreviation	Explanation
RQ	Risk quotient
SCB	Statistiska centralbyrån (Official Statistics of Sweden)
SOP	Standard operating procedure
SRT	Sludge retention time
SSD	Species sensitivity distribution
STP	Sewage treatment plant
TGD	Technical guidance document (EU, 2003)
TM	Technical meeting
TNO	Nederlandse Organisatie voor Toegepast Natuurwetenschappelijk Onderzoek (Netherlands Organisation for Applied Scientific Research)
TNsG	Technical Notes for Guidance
TWA	Time-weighted average
UBA	Umwelt Bundesamt (Federal Environment Agency of Germany)
UNEP	United Nations Environment Programme
UVCB	Undefined or variable composition, complex reaction products or biological material
UWWTD	Urban Waste Water Treatment Directive (UWWTD, 91/271/EEC)
WAF	Water accommodated fraction
WWTP	Waste water treatment plant

1. Introduction

Regulation (EU) 528/2012 in the following referred to as "BPR" requires that an environmental risk assessment on the active substance present in the biocidal product must always be carried out. If there are, in addition, any substances of concern present in the biocidal product then a risk assessment must be carried out for each of these. The risk assessment must cover the proposed normal use of the biocidal product, together with a realistic worst-case scenario including any relevant production and disposal issue. The assessment must also take account of how any "treated articles" treated with or containing the product may be used and disposed of. As the provisions for treated articles are new for biocides, specific descriptions on treated articles were added (in Section 2.3.3.2 of this Guidance). Active substances that are generated in-situ and the associated precursors must also be considered. The risk assessment must entail:

- **Hazard identification**: the identification of the adverse effects which a substance has an inherent capacity to cause
- **Dose (concentration) - response (effect) assessment** (as appropriate): the estimate of the relationship between the dose, or level of exposure, of an active substance or a substance of concern in a biocidal product and the incidence and severity of an effect
- **Exposure assessment**: the determination of the emissions, pathways and rates of movement of an active substance or a substance of concern in a biocidal product and its transformation or degradation in order to estimate the concentration/doses to which environmental compartments are or may be exposed
- **Risk characterisation**: the estimation of the incidence and severity of the adverse effects likely to occur in environmental compartments due to actual or predicted exposure to any active substance or substance of concern in a biocidal product. This may include "risk estimation" i.e. the quantification of that likelihood.

The risk assessment must take account of any adverse effects arising in any of the environmental compartments sewage treatment plant (STP), air, soil (including groundwater) and water (freshwater and marine, including sediment), i.e. aquatic environment (including sediment). Where quantitative results are not available the results of the qualitative assessments must be integrated in a similar manner.

The present document is intended to assist applicants and competent authorities to carry out the environmental risk assessment of active substances, their metabolites (if relevant) and substances of concern in a biocidal product or in a treated article (in the following, these are subsumed under the term "substance").

This guidance document includes advice on the following issues:

- how to calculate Predicted Environmental Concentrations (PECs) (Sections 2 and 4.2 of this Guidance)
- how to calculate Predicted No-Effect-Concentrations (PNECs) (Sections 3 of this Guidance) and,
- where the calculation of PECs and PNECs is not possible, how to make qualitative estimates of environmental concentrations and effect/no effect concentrations
- how to calculate the PEC/PNEC ratio (Section 4 of this Guidance)
- how to assess exclusion criteria, including how to conduct a PBT/vPvB assessment and how to assess endocrine disrupting properties assess (Section 3.11 of this Guidance)

- how to assess aggregated exposure (Section 4.7 of this Guidance);

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 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 Section 4.5 of this Guidance.

The risk assessments that have to be carried out according to the BPR are in principle valid for all countries in the European Union. Therefore, in the first stage of the exposure assessment, where exposure models are used, so-called generic exposure scenarios are applied in this document. 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. It is recognised, however, that exposure estimation, for example, is subject to variation due to topographical and climatological variability. 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.

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.

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 4.4 of this Guidance).

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 biocides 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 (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.

At present, the environmental risk assessment methodology has been developed for the following compartments:

For inland risk assessment:

- aquatic ecosystem (including sediment);
- terrestrial ecosystem (including groundwater);
- 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 (primary/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.

The PECs can be derived from model calculations and/or available measured data. When using measured data to derive a PEC care should be taken to ensure that the measured data is sufficiently representative of a reasonable worst case exposure level across the EU. This will ensure that the level of protection afforded by the assessment using measured data is consistent with that based on model calculations. Please refer also to Section 2.4 of this Guidance.

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.

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.

In some cases, the current quantitative risk assessment approach does not provide sufficient confidence that the environmental compartments considered are sufficiently

protected. The PBT assessment, to which is referred to in Section 3.11 of this Guidance, 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 Table 1 and Table 2, several other exposure levels are derived in Section 2 of this Guidance. These are used for the assessment of indirect human exposure through the environment, which is described in Volume III, Part B (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	Section	PNEC	Section
Aquatic organisms	Surface water	2.3.8.3	$PNEC_{water}$	3.3
Benthic organisms	Sediment	2.3.8.4	$PNEC_{sed}$	3.5
Terrestrial Organisms	Agricultural soil	2.3.8.5	$PNEC_{soil}$	3.6
Fish-eating Predators	Fish	3.8	$PNEC_{oral}$ from $NOAEL_{avian/mammalian}$	3.8
Worm-eating Predators	Earthworms	3.8	$PNEC_{oral}$ from $NOAEL_{avian/mammalian}$	3.8
Microorganisms	STP aeration tank	2.3.7	$PNEC_{stp}$	3.4

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

Target	Exposure scenario	Section	PNEC	Section
Aquatic organisms	Seawater	2.6.5.2	$PNEC_{seawater}$	3.9.1.3
Benthic organisms	Seawater sediment	2.6.5.3	$PNEC_{seased}$	3.9.2.4
Fish-eating predators	Fish	3.9.3	$PNEC_{oral,\ predators}$	3.9.3
Top predators	Fish-eaters	3.9.3	$PNEC_{oral,\ top\ predators}$	3.9.3

Table 3: Exposure levels used for indirect human exposure

Target	Exposure scenario	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. Exposure assessment

2.1. Introduction

According to the BPR Annex VI, exposure assessment comprises of the determination of the emissions, pathways and rates of movement of an active substance or a substance of concern, in a biocidal product or in a treated article, and its transformation or degradation in order to predict their likely concentration in the environment, which is known as predicted environmental concentration (PEC). However, in some cases it may not be possible to establish a PEC and a qualitative estimate of exposure has then to be made.

A PEC, or where necessary a qualitative estimate of exposure, need only be determined for the environmental compartments to which emissions, discharges, disposal or distributions (including any relevant contribution from articles treated with biocidal products) are known or are reasonably foreseeable.

The PEC, or the qualitative estimation of exposure, must be determined taking account of, in particular and where appropriate:

- adequately measured exposure data;
- the form in which the product is marketed;
- the type of biocidal product/treated article;
- the application method and application rate;
- the physico-chemical properties;
- breakdown/transformation products;
- likely pathways to environmental compartments and potential for adsorption/desorption and degradation;
- the frequency and duration of exposure;
- the size of the receiving compartment;
- long range environmental transportation.

When conducting the exposure assessment, special consideration should be given to adequately measured, representative exposure data where such data are available. Where calculation methods are used for the estimation of exposure levels, adequate models should be applied. Where appropriate, on a case-by-case basis, relevant monitoring data from substances with analogous use and exposure patterns or analogous properties should also be considered.

The assessment of environmental exposure consists in more detail of:

- the estimation of emissions into the different environmental compartments air, water (fresh- and seawater), sediment (fresh- and seawater), soil (including groundwater) and sewage treatment plant;
- the assessment of the degradation and transformation processes;
- the assessment of distribution over the different compartments;

- the exposure of organisms within those compartments, either directly or indirectly via the food chain.

The environment may be exposed to biocides during all stages of their life-cycle from production to disposal or recovery. However, for biocides only certain life-cycle stages are assessed in line with Article 2 of the BPR since it is assumed that the other stages are covered by other legislations. The life-cycle stages for biocides to be covered by a quantitative risk assessment are highlighted in the following list **in bold letters**. The life-cycle stage for biocides (see also Figure 2 below) for which no quantitative assessment is needed (in particular production and waste disposal) should nevertheless be covered at least by a qualitative assessment:

- production (of an active substance);
- **formulation** (of an active substance in a biocidal product)[1];
- **application/use:**
  - **industrial/professional** (large scale use including processing (e.g. industry) and/or small scale use (e.g. trade or trained experts));
  - **private or consumer;**
- **service life;**
- waste disposal (including waste treatment, landfill and recovery).[2]

For each environmental compartment potentially exposed, the exposure concentrations should be derived.

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 a substance related to the use of a biocidal product is given in Section 4.6 of this Guidance.

In view of uncertainty in the assessment of exposure of the environment, the exposure levels should be derived on the basis of both model calculations and measured data, if available. 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 2.2.2 and 2.4).

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. 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 Appenix 3. Furthermore it should be noted that guidance on how to assess and test relevant metabolites and transformation products is available for plant protection products and can be used also for biocides (see Appendix 6).

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[1] Relevant for active substances used in treated articles, formulation of disinfectants, preservatives, repellents and insecticides into the end-product to be preserved

[2] This step is considered quantitatively only in the exposure assessment for product-type 13.

Infobox 1: Metabolites

A difference is made between:

Major metabolite: In Volume IV A, Part 1 it is stated that major metabolites (formed ≥ 10% on a molar basis, of the active substance in any relevant environmental compartment or appear at two consecutive sampling points at amounts ≥ 5% on a molar basis, or if at the end of the study the maximum of formation is not yet reached but accounts for ≥ 5% on a molar basis, of the active substance at the final time point), should be identified and their behaviour and toxicity should be assessed. In general, an environmental risk assessment for the relevant compartments needs to be performed for all major metabolites. However, as a first step a semi-quantitative assessment of these metabolites using the available data and expert judgement to fill data gaps may be sufficient. A quantitative assessment should be performed on a case-by-case basis.

Minor metabolite: metabolites that are no major metabolites.

Ecotoxicologically relevant metabolite: a metabolite which poses a higher or comparable risk to aquatic or terrestrial organisms as the active substance.

Fate and ecotoxicological studies are required for all **major** metabolites and a risk assessment should be performed. Furthermore, the 'specifics' of biocides should be taken into account.

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 e.g. manure 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 or POP profile[3]. 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.

2.2. Exposure assessment principles

2.2.1. Assessment scale

The exposure to the environment is in principle assessed for biocides only on the local scale, i.e. in the vicinity of point sources of release to the environment.

The regional scale covers a larger area that includes all point sources and wide dispersive sources in that area. Releases at the continental scale are considered to provide inflow concentrations for the regional environment. However, regional (and continental concentrations) are used as endpoints in the exposure assessment of biocides only case by case, for example for treated articles.

For the **local assessment**, concentrations of substances released from a single point source 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" and a standard town of 10,000 inhabitants (including a standard

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

sewage treatment plant). The exposure targets are assumed to be exposed in, or at the border of the site. In general, concentrations during an emission episode are measured or calculated. This means that local concentrations (PEC_{local}) are calculated on the basis of a daily release rate, regardless of whether the discharge is intermittent or continuous. They represent the concentrations 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 average is used instead of daily release rates. This is because exposure is assumed not to be influenced by temporal fluctuation in release rates. 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 calculation of the PEC_{local}. However, because of the relatively short time between release and exposure, concentrations at local scales are mainly controlled by initial mixing (dilution into environmental compartment) and adsorption on suspended matter.

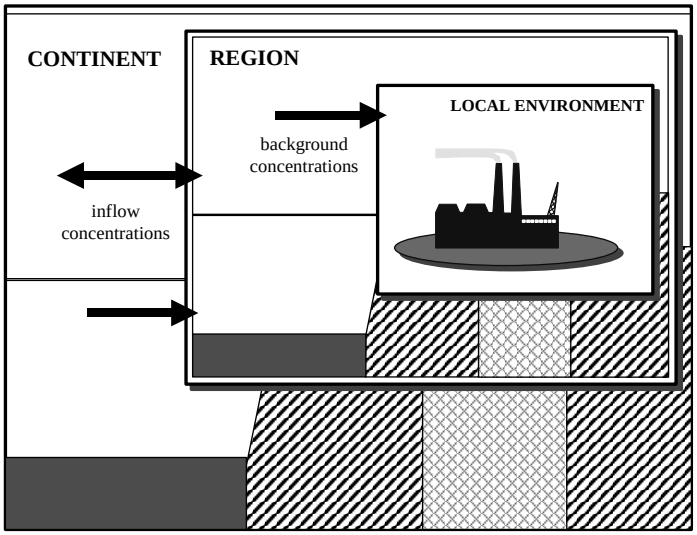
A fixed dilution factor of 10 is applied to the effluent concentration of an STP (by default assumed to be present). For further iterations, more specific assessments may be appropriate. The actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate of the STP. This approach should be used for rivers only and not for estuaries or lakes. In other cases, the calculation of the PEC_{local} can be carried out using actual environmental conditions around the point source.

Release to the environment at the local scale can be from private settings (e.g. painted houses), industrial settings or from wide dispersive uses:

- Releases from uses in **private** and **industrial settings** are assessed as independent point source releases; it means that each identified use of the substance is assumed to occur at a different site. However, in some cases those assessments are combined (e.g. for product-type 6: preservatives for products during storage', for certain treated articles or for product-type 18: insecticides, acaricides and products to control other arthropods and for certain treated articles). Releases to water can be treated in an on-site industrial waste water treatment plant (WWTP) or in a municipal sewage treatment plant (STP). For industrial or municipal biological treatment plants, a standard model is available to calculate the releases after treatment (Section 2.3.7 of this Guidance). Indirect releases to air via the STP, as a result of water treatment in the STP, are also considered. Release to soil at the local scale will occur via application of sludge from an STP to agricultural soil[4] and via atmospheric deposition of substances released to air. Direct releases to soil or surface water from private settings are only relevant for specific uses of certain product types (PT) (e.g. product-type 8: direct release during painting a fence/house). Guidance on how to perform the assessment of direct releases is provided in the PT-specific emission scenario documents (ESDs), see also Section 2.3.3.3.1. of this Guidance.

[4] It should be noted that sewage sludge is not applied as a soil fertiliser in many European countries, but fermented and eventually burned as hazardous waste. Exposure to soils via sewage sludge is therefore not relevant in many European countries.

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



- A **wide disperse use** of a substance is characterised by the assumption that the substance is used by consumers or by many users in the public domain, including small, non-industrial companies. A wide dispersive use of a substance is by default associated with a point source release of a local municipal STP of a standard 10,000-inhabitant town that collects the releases to water from that use. This is not the case for direct releases to air and soil from wide dispersive uses.

On the **regional scale**, concentrations of substances released from point and diffuse sources over a wider area are assessed for a generic regional environment. The $PEC_{regional}$ 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 PEC_{local}. As with the local models, a generic standard environment is defined. The $PEC_{regional}$ 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.

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.

2.2.2. Measured / calculated environmental concentrations

No measured environmental concentrations will normally be available for new active substances. Therefore, concentrations of a substance in the environment must be estimated. In contrast, the exposure assessment of existing active 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).

In many cases, a range of concentrations from measured data or modelling will be obtained. This range can reflect different conditions during use or service life 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.

Initially, a generic "reasonable worst-case" exposure assessment based on modelling should be performed, to derive an 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 e.g. effluent volumes, size of STP, river flow. may also be useful. In carrying out this revision, it is recommended to include in the exposure assessment of active substances, a table containing availability of site-specific information for industrial sites (if limited in number) or group of industrial 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). It should then be considered 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 grounds on which the extrapolation has been done should be justified in the risk assessment. 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 this document should be followed for the (group of) site(s).

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 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 2.4 of this Guidance 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 of this Guidance discusses modelling in detail. Section 2.5 of this Guidance gives further advice on critical comparison between calculated and measured PECs.

2.3. Model calculations

2.3.1. Introduction

The first step in the calculation of the PEC is to evaluate the data set. The subsequent step is to estimate the substance's release rate based on its use pattern. All potential emission sources need to be analysed, and the releases and the receiving environmental

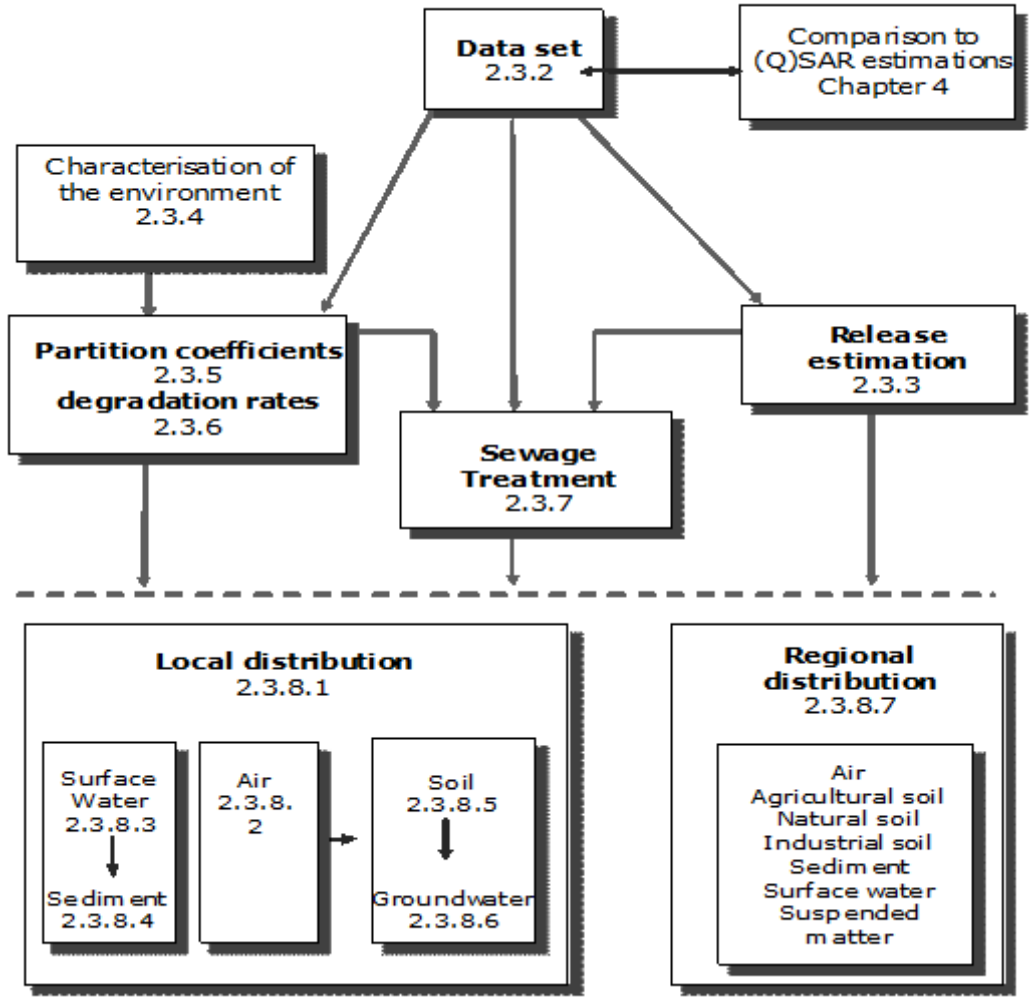
compartment(s) identified. After assessing releases, the fate of the substance once released to the environment needs to be considered. This is estimated by considering likely routes of exposure and biotic and abiotic transformation processes. Furthermore, secondary data (e.g. partition coefficients) 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 PEC values in the receiving compartments. The PEC calculation is not restricted to the primary compartments; surface water (Section 2.3.8.3 of this Guidance), soil (Section 2.3.8.5 of this Guidance) and air (Section 2.3.8.2 of this Guidance); but also includes secondary compartments such as sediments (Section 2.3.8.4 of this Guidance) and groundwater (Section 2.3.8.6 of this Guidance). 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 emissions to the environment;
- definition of the characteristics of the standard environment used in the estimation of PECs;
- 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;
- distribution and fate in the environment, and estimation of PECs.

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: Layout 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 reference to a table with defaults]
[Symbol]	[Description of resulting parameter]	[Unit]	

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·d^{-1}]
F	for dimensionless fractions	[kg·kg^{-1}] or [m^3·m^{-3}]
C	for the concentration of a substance	[mg·l^{-1}], [mg·kg^{-1}] or [mg·m^{-3}]
RHO	for densities of compartments or phases	[kg·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 $F_{oc,\ soil}$ means the fraction (*F*) of 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 most appropriate input parameter should be selected according to the "realistic worst case" scenario being assessed and should be used in the "core assessment". In most cases, the vulnerability of the realistic worst case scenario will be a result of the choices of realistic worst case default scenario assumptions. In such cases it will often be appropriate to use average, median or geometric mean substance specific input parameters rather than worst case values to avoid the overall assessment being overly conservative. The use of average input values will generally be appropriate when the full active substance or metabolite information requirements have been fulfilled. In all cases the selection of substance specific input parameters should be detailed and justified as part of the exposure assessment. Alternative input values should only be included in alternative estimations performed for investigation purposes. Alternative input parameters (e.g. worst case values) may be justified when the full information requirements have not been fulfilled to ensure an appropriately conservative assessment is performed.

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 core data set (CDS) are directly used in the exposure models as discussed in the following sections:

Physico-chemical properties

MOLW	molecular weight	[g·mol^{-1}]
K_{ow}	octanol water partitioning coefficient[5]	[-]
SOL	water solubility	[mg·l^{-1}]
VP	vapour pressure	[Pa]
BOILPT	boiling point (only for some release estimations)	[°C]

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/b for ionising substances) may be required for other types of substances. For ionising substances, the pH-dependence of K_{ow} and water solubility should be known. Partition coefficients should be corrected according to the pH of the environment and the effect across a typical environmental range should be investigated (e.g. the influence on partitioning across pH 4 to 9).

The correction can be done by using the following correction factor (see also Section 4.5.3 of this Guidance):

$$CORR = \frac{1}{1 + 10^{A(pH - pKa)}} \quad (1)$$

Explanation of symbols

A	1 for acids, -1 for bases	
pH	pH value of the environment	
pKa	acid/base dissociation constant	data set

Equation 1 results in the fraction of undissociated compound for the proton donating (acidic) reactions for an acid:

$AH \rightarrow A^- + H^+$ with the value for A = 1;

or for a base:

$BH^+ \rightarrow B + H^+$, with the value of A = -1.

This equation is only valid for monoprotic substances.

[5] The term K_{ow} is used in this document and is equivalent to Pow.

If the sorption behaviour has been investigated for a substance over a relevant pH range, the measured value should be used preferably over the use of the above equation. In this case, the most applicable (worst case) measured K_{oc} or Kom for the compartment to be considered should be selected, which may result in the use of different K_{oc}/K_{om} values for respective compartments (e.g. the use of different values for groundwater and sediment).

For surface active substances specifically, and for substances for which adsorption and partition is not related to binding to organic matter in general, it may not be advisable to use estimated or measured K_{ow} values as a predictor for e.g. K_{oc} (soil, sediment, suspended organic matter and sludge) and BCF (fish, worm) because the predictive value of log K_{ow} for such estimations may be too low. Instead, for surfactants it may be appropriate to obtain measured K_p 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 relevant temperature of the exposure models employed (e.g. 12 °C in the regional model or 9 °C for marine environments) then such an extrapolation should be considered. In other cases this will not be necessary. Particular care is also required for the interpretation of test results for thermolabile substances.

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:

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

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 liquid is always higher than of the solid ('fugacity ratio' see equation 20). Extrapolation will therefore tend to overestimate the vapour pressure. There is no general solution to this problem. One approach to overcome the problem is to use K_{ow}, Koctanol-air, and Kair-water instead of the 'three solubilities' (vapour pressure water solubility, solubility in octanol), as discussed in equation 20.

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

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

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	$[Pa \cdot m^3/(mol \cdot K)]$	8.314

2.3.3. Release estimation

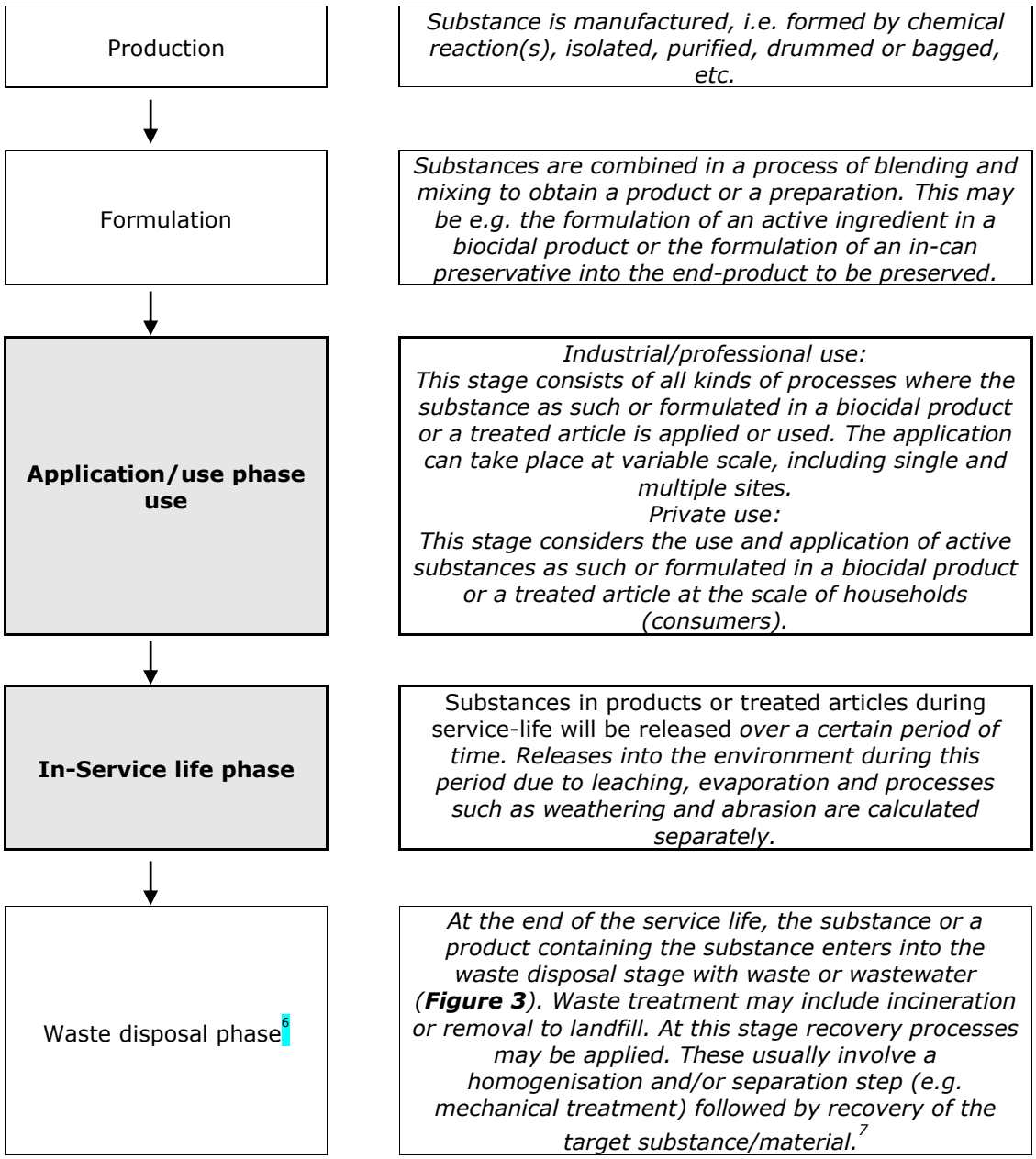
In this section the following parameters are derived:

- local emission, the rates to air and wastewater during an emission episode;
- regional emissions to air, wastewater, and 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 (see **Error! Reference source not found.** below). However, emissions rom substance production, and product formulation are considered less relevant (since potentially covered by other legislations) compared to emissions from the application- and in service phase of the product. For the application- and in service phases, the emission routes should be identified and be assessed. The exposure assessment must cover the proposed normal use of the biocidal product or treated article together with a realistic worst-case scenario. Determination of the relevance of the emission routes and quantification of emissions are based on emission scenarios that have been drawn up for various product-types (see section 2.3.3.3.1 of this Guidance).

Figure 3: Schematic representation of the life cycle stages of a substance



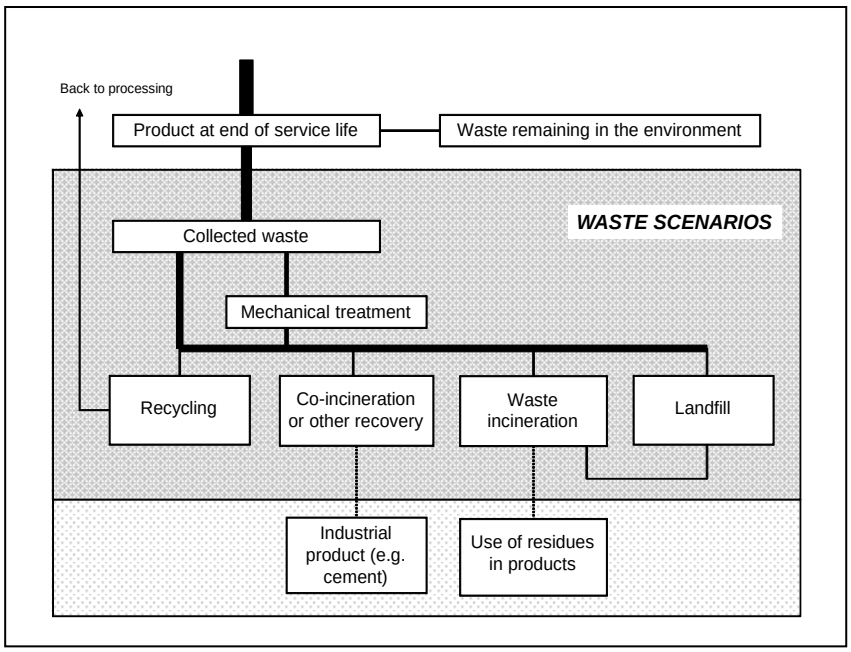
[6] This step is considered quantitatively only in the exposure assessment for product-type 13.

[7] The recovered substance or material may be:

- reprocessed for the original type of product (recycling) - the substance returns into life-cycle stages already assessed before
- manufactured into a new type of product;
- used as secondary fuel in heat production.

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.
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.
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

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



2.3.3.2. Types of emissions, sources and emission pathways

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 noise barrier). Releases may also be continuous or non-continues like peak or block emissions. The latter can be also intermittent (see also section 2.3.3.4 of this Guidance). 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 preservation process such as in cooling towers). 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 disinfectants in a batch disinfection process e.g. in food production industry). Block emissions are characterised by a flow rate which is reasonably constant over certain time periods with regular intervals (e.g. the emissions form harbours during the application and removal phase of antifouling to boat hulls at the beginning of the sailing season sailing). 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 applied in closed systems.

Besides releases from point sources, diffuse emissions from treated 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 (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).

Infobox 2: Emission pathways of biocides and receiving environmental compartments

The **STP** can be exposed to releases from indoor applications in industrial, public and private areas (e.g. indoor use of surface disinfectants) as well as by releases from outdoor applications (e.g. leaching from a noise barrier, treated with a wood preservative).

The substance may be released from the STP to the following consecutive environmental compartments:

STP → Water → Sediment (sea/freshwater)
STP → Air → Soil
STP → Soil → Groundwater

Water (freshwater or seawater) can be either a direct recipient (e.g. from outdoor spray applications against insects or by leaching from e.g. antifouling agents applied on ships) or can be exposed indirectly via the effluent from an STP that contains residues.
The consecutive environmental compartment is freshwater- or seawater sediment.

Soil can receive direct emission of the active substance during application or service life of a biocidal product (e.g. emissions during outdoor in-situ applications or leaching from a house treated with wood preservatives) or indirect emissions from application of residue-containing sludge from an STP or manure from treated animal housings.

Emissions to soil result in the exposure of the following consecutive environmental compartments:

Soil → Groundwater
Soil → Surface water (not routinely assessed)

Air is exposed if a product contains volatile active substances or by direct emissions from aerosols or spray applications. Direct emission can also occur from evaporation and drift containing biocidal preservatives e.g. used in cooling systems (PT 11).

Emissions to air result in exposure of the following consecutive environmental compartments:

Air → Soil (through deposition)
Air → Water (through deposition, not routinely assessed) → Sediment

There are two main routes of exposure to **birds and mammals**; primary and secondary exposure. Primary exposure means that birds or mammals are either directly in contact with the substance (e.g. contact to rodenticides) or they are directly exposed via an environmental compartment to which the substance was released.

Secondary exposure entails the exposure to a substance through the natural food chain where the food of birds or mammals contains substances or their metabolites. In general, secondary exposure is assessed if 1) the substance has a high bioaccumulation potential and 2) the toxicity of the active substances to birds is high. For most organics, a cut off value of log K_{ow} of 3 is used to indicate the bioaccumulation potential. However, this cut off value of log K_{ow} is based on a QSAR and not all organic substances are suitable for this QSAR.

Exposure from treated articles

Articles treated with or incorporating biocidal products can lead to consumer and environmental exposure if chemical constituents of the active substances are released in any way. Exposure from treated articles during service life may be the most significant exposure to the active substance. Specifically, articles consisting of different types of polymers can be used in a large range of consumer applications, which makes the exposure situation very complex. Such applications also can belong to a wide range of product types (PTs). The diversity of applications has consequences for the exposure of the environment. Uses with similar exposure patterns (e.g. down the drain, direct

exposure to soil, etc.) should be summed up in an aggregated exposure assessment (see section 4.7 of this Guidance).

When treated articles are imported into the EU, the only possible way to carry out a risk assessment is by active substance evaluation. The risk assessment of the intended uses in treated articles is therefore to be included in the Competent Authority Report (CAR).

Definitions

The ***use*** of the biocidal product can include the application of the biocidal product itself (professional or amateur use), the formulation of a treated article (e.g. conversion and compounding of plastic materials; spraying, dipping, thermal impregnation, etc. for wood) as well as the use of the treated article itself (e.g. painting a façade with an outdoor paint containing an algicide or fungicide).

Service life: Use of a treated article in service, e.g. treated wood on a children's playground, a painted façade; shower curtains, fillers, treated kitchen tops, treated apparel, etc. in use (see also chapter 2.1).

Environment

Due to the diversity of uses in treated articles, the exposure has to be related to both the PTs and the specific use of the treated article. Both of these are needed to describe the exposure pattern. For use in treated articles, besides the properties of the active substance, more aspects have to be taken into account:

- physical condition of the treated article (solid, liquid). This can change during different use phases (e.g. for paints and coatings);
- material the treated article consists of and the structure of the material (wood, plastic, hard or porous surface);
- duration of the service life of the treated article and possible accumulation in the technosphere (see also chapter 2.3.3.5);
- use pattern of the treated article (open space, outside under roof, in-house, in contact with water/soil; regular washing, occasional wiping, etc.).

It is important to consider which of these parameters have effects on the exposure situation. As it is impossible to take into account every single use in detail, it is necessary to summarize similar uses to exposure categories (e.g. regularly washed textiles, treated wood exposed to rain and in contact with soil). It can also be meaningful to estimate which uses probably will have a big impact on the emission situation for a certain compartment (e.g. regularly washed treated textiles) and which uses probably have a small impact (e.g. articles used in-house and wiped occasionally). If the variety of possible uses cannot be handled otherwise, focus should be laid on the uses with a big impact. The REACH guidance on the estimation of exposure from articles (*Guidance on information requirements and chemical safety assessment. Chapter R.17: Estimation of exposure from articles*), is very comprehensive and can be applied in many cases. Also the OECD Guideline document on how to write emission scenarios for the life-cycle step service life can be of help.

To estimate the exposure from treated articles, it might be the easiest way forward to apply the tonnage approach. As a default, the whole tonnage of the active substance, possibly from different suppliers, is used for the emission calculations. The different shares of the tonnage then have to be allocated to the different use patterns or exposure categories. The notifier of the active substance has to help with these allocations. In case the tonnage approach is not used, typical concentrations of the active substance have to be considered for each use and a quantitative estimation of the amount of treated material/articles with a certain use-pattern (e.g. antimicrobial/anti-fungal treated floors in public buildings) has to be made. Possibly, different concentrations of the active substance

for different use patterns or different parts of the EU/EEA have to be taken into account (e.g. for treated wood). To consider the different fields of use, use patterns, concentrations of the active substance in a material and different leaching rates from different materials are a precondition for a realistic estimation of environmental exposure of the active substance. Information on the estimated life time of the treated article and possible re-applications, if relevant, are necessary.

Leaching

In higher-tier estimations, leaching rates out of the treated article can be applied to refine the exposure estimations. The assessment can be based on model calculations with well supported default values and/or measured laboratory leaching values, or based on the results of a field or semi-field exposure study. It is important to consider different types of materials/uses which may show different leaching patterns. The duration of the field- or semi-field study should reflect the exposure situation and enable an extrapolation to the service life of the treated article. For polymers, it has to be taken into account that leaching rates can vary quite significantly depending on the type of polymer (e.g. polyethylene leaches less than polyamide, etc.), the type of application (incorporation or coating) and of the use (a regularly washed textiles leaches much more than a kitchen worktop). For wood preservatives, guidance on extrapolation of leaching rates for life time calculations can be found in part 3 of the Emission Scenario Document for PT 8 (OECD, 2009).

No reliable method exists to predict the leaching rate based on physico-chemical properties of the active substance and therefore leaching studies are normally required. In general a tiered approach should be followed:

- Tier 1: worst-case assumption where 100% of the active substance is assumed to leach after a given time. The life time can be different and depends on the PT and use of the treated article. For polymers, default values of life time of different consumer articles are given in the OECD Emission scenario document on plastic additives.
- Tier 2: validated laboratory leaching test. The uncertainty of using a laboratory test to predict environmental concentrations should be addressed by using an assessment factor.
- Tier 3: semi-field tests or monitoring studies.

For some PTs like e.g. PT 2, 4, 7, 9, and 10, the biocidal product is often added as a premix concentrate to a polymer. The polymer may subsequently be applied to a surface and/or incorporated into a matrix from which leaching of the active substance(s) will take place. As these surfaces/matrices may have many different characteristics, it is important to take into account data for the leaching behaviour for different types of surfaces/matrices which is likely to cover the worst-case leaching behaviour.

The emissions during service life are considered to be diffuse emissions that usually cause exposure on a regional scale. In some cases, however, local exposure scenarios should also be considered. Examples of local scenarios are e.g. wood preservatives or other substances leaching from construction materials, as described in the ESDs for PT 8, 10 and in the Guidance note on leaching rate estimations for substances used in biocidal products in PT 07, 09 and 10 of 2010 (endorsed at the 36th CA meeting). Emissions of the diffuse/wide dispersive type have to be summed up in an aggregated exposure scenario. Possible environmental emissions from articles treated with the same active substance should be summed up. Exposure categories, i.e. uses with the same emission pattern, can be helpful to simplify the aggregated exposure assessment.

Exposure from the waste stage of the treated articles should also be taken into account, if relevant. For this, the *Guidance on information requirements and chemical safety*

assessment Chapter R.18: Exposure scenario building and environmental release estimation for the waste life stage can be applied.

Further guidance:

- Guidance on information requirements and chemical safety assessment. Chapter R.17: Estimation of exposure from articles (http://echa.europa.eu/documents/10162/13632/information_requirements_r17_en.pdf)
- Guidance on information requirements and chemical safety assessment. Chapter R.18: Exposure scenario building and environmental release estimation for the waste life stage (http://echa.europa.eu/documents/10162/13632/r18_v2_final_en.pdf)
- Guidance note on leaching rate estimation of PT 07, 09 and 10, (http://ihcp.jrc.ec.europa.eu/our_activities/public-health/risk_assessment_of_Biocides/doc/TNsG/Guidance_leaching_rate_PT_07_09_10.pdf)
- Workshop on determination of the leaching rate for PT 08, (http://echa.europa.eu/documents/10162/16908203/pt8_leaching_workshop_2005_en.pdf)
- OECD 313 (2007), CEN/TS 15119-2 (2008) treated wood, use class 4, (http://ihcp.jrc.ec.europa.eu/our_activities/public-health/risk_assessment_of_Biocides/doc/ESD/ESD_PT/PT_08/PT_8_Wood_preservatives_3.pdf/view)
- OECD TG 107 (2009) Treated wood, use class 3, (http://echa.europa.eu/documents/10162/16908203/pt8_oecd_guidance_emission_estimation_treated_Wood_en.pdf)
- OECD (2013): OECD SERIES ON EMISSION SCENARIO DOCUMENTS Number 2: Revised Emission Scenario Document for Wood Preservatives, (http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents)
- OECD (2009): OECD SERIES ON EMISSION SCENARIO DOCUMENTS Number 3: EMISSION SCENARIO DOCUMENT ON PLASTIC ADDITIVES; ENV/JM/MONO(2004)8/REV1 revised 2009 (http://search.oecd.org/officialdocuments/displaydocumentpdf/?cote=env/jm/mono(2004)8/rev1&doclanguage=en)
- OECD (2009): OECD SERIES ON EMISSION SCENARIO DOCUMENTS Number 19: COMPLEMENTING GUIDELINE FOR WRITING EMISSION SCENARIO DOCUMENTS: THE LIFE-CYCLE STEP "SERVICE-LIFE" (http://search.oecd.org/officialdocuments/displaydocumentpdf/?cote=env/jm/mono(2008)41/rev1&doclanguage=en)

2.3.3.3. Emission estimation

Emission estimation applies either the tonnage of the substance or the average consumption/application rate as a starting point. In both cases emission factors (fractions released to the relevant environmental compartments) are used. Information on when to apply what type of calculation (i.e. tonnage or consumption based) and on emission factors is provided in the following chapters.

2.3.3.3.1. Consumption/application rate based approach

The consumption/application rate based approach is based on the quantity of a substance used in a single application or treatment. The application or dose rate of a substance is multiplied by the treatment area or volume or any other relevant unit or measure.

Emission Scenario Documents (ESDs) provide default values per product-type[8] for the treatment areas and volumes or use rate such as e.g.:

- dimensions of external façade (range of scenarios) for the outdoor use of masonry/wood preservatives/paints;
- area treated (crack & crevice, barrier treatment, ant nest etc.) for indoor and outdoor use of insecticides;
- quantity used per person per day for the consumer use of disinfectants/personal care products.

The consumption/application rate based approach is particularly suited to situations where exposure is highly localised such as direct or indirect emission to soil. Further advantages of this approach are that it is standardised due to the ESDs, it is suited to point sources and it can be communicated in a transparent way.

The disadvantages are that emission estimations concern the local scale only although background contribution can be significant when a large number of uses is to be considered, they require a good understanding of the application, for some default values there is a lack of reliable data and there is no direct relation with the actual volume for the application. In addition the conduction of an aggregated exposure assessment is difficult.

Emission Scenario Documents:

For the emission estimation of most of the PTs respective ESDs and additional related documents are available which are provided on the ESD specific ECHA webpage: http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents).

In the following Table 4 specific calculations provided in the ESD or additional related document for one PT relevant also for other PTs are summarised.

Table 4: Overview on specific calculations in the ESD with relevance for other PTs

PT	Description	Methodology providedin PT-specific ESD with relevance for other PTs
PT 3	Veterinary hygiene	Release to manure/slurry in animal housing Application of manure/slurry to arable- or grassland based Nitrogen/phosphate standards for manure/slurry application
PT 5	Drinking water	Degradation in the sewer system (relevant for rapidly degrading or oxidising substances)
PT 8	Wood preservatives	- Degradation in the environmental compartments soil, surface water and sediment (after direct release) - Groundwater exposure assessment, i.e. simulation (following leaching) - Soil studies applicability for mobile or persistent substances and DT_{50}/Koc input values for PELMO/PEARL models

[8] Product type as specified inBPR Annex V

PT	Description	Methodology providedin PT-specific ESD with relevance for other PTs
PT 10	Construction material preservatives	Urban scenario (leaching from a house and emission to the STP)
PT 11	Preservatives for liquid-cooling and processing systems	Evaporation, deposition from air (cooling tower)
PT 12	Slimicdes	CHARM Model
PT 13	Working or cutting fluid preservatives	Waste stage, - Special STP
PT 14	Rodenticides	Assessment of primary poisoning and secondary poisoning
PT 18	Insecticides, acaricides and products to control other arthropods	See PT3 Assessment of secondairy poisoning via consumption of insects, vegetation and worms (Household Professional use)
PT 21	Antifouling products	MAMPEC (sediment) Wider environment

Product-type specific amendments to the ESDs:

In the course of the ongoing review program for biocides, decisions were taken for several PTs which specify the emission estimation and should be taken into account when preparing an exposure assessment. These decisions have first been published in the Manual of technical agreements (MOTA) version 6 and are now included in the Technical Agreememts for Biocides (TAB) available on the ECHA Websit.

2.3.3.3.2. Tonnage based approach

The tonnage based approach takes into account the annual EU tonnage and it is primarily focused on emission to wastewater. In the emission estimation a fraction of the annual EU tonnage is defined which is used in a standard EU region (F_{region}) and a standard STP catchment ($F_{mainsource}$). The daily emission is then determined by taking account of number of emission days ($T_{emission}$).

The advantages of the tonnage based approach are that no use details are required, the tonnage will be known to the applicant, the emission is related to the used volume and it facilitates the conduction of an aggregated assessment.

The disadvantages are that tonnage data are confidential, the representation for a long term view is questionable (growth, share etc.), it is not suitable to cover direct emissions to soil and water and it bears a certain uncertainty with regard to the distribution of uses.

The tonnage based approach is described in several ESDs (e.g. ESD for PT 1 and PT 2). However it was developed for industrial chemicals and was originally described in the TGD of 2003. Since the text from the TGD (2003) is still relevant for this approach, the original text from the TGD is provided in the following (beside adapted Appendix/Annex numbers) The examples provided in the original text have been revised in order to be more specific for biocides.

Tonnage based approach (cited from TGD 2003):

Emissions 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 Appendix 7 of Vol. IV Part B. 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 and service life). 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 as preservative in a closed cooling circuit,
- 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 e.g. as an in-can preservative 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. 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:

- specific information for the given substance (e.g. from producers, product registers or open literature);
- specific information from the ESDs which are available for most of the 22 PTs;
- emission factors as included in the release tables of Appendix VII

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 7, 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 7 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 $PEC_{regional}$ calculation.

The B-tables of Appendix 7 are used for the determination of the releases from point sources for the evaluation of PEC_{local}. 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 Industrial catergory/Use category (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 active 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.

In general, the data supplied by industry will help to find the correct entry to the release tables Appendix 7

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 7, 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 of substance	[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 7 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 (not relevant for biocides)	a	air
2	Formulation (only relevant for the formulation of the biocidal product into an end-product)	w	water
3	industrial/professional use	s	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 7, and the releases, which are the output from emission tables and the calculation routine of Appendix 7.

Input

MAINCAT	main category (for substances)	[-]	data set
INDCAT	industrial category	[-]	data set
USECAT	use category	[-]	data set
TONNAGE	tonnage of substance (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. 7
Fmainsource$_i$	fraction of release at the local main source at life-cycle stage *i*	[-]	App 7
Temission$_i$	total number of days for the emission at life-cycle stage *i*	[d]	App. 7

For each stage other than production, the losses in the previous stage are taken into account (see calculation in Appendix 7). 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%. It must be specified 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 of this Guidance).

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 of this Guidance).

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. 7
$F_{mainsource,\ i}$	fraction of release at the local main source at life-cycle stage *i*	[-]	App. 7
$T_{emission,\ i}$	number of days per year for the emission in stage *i*	[d·yr^{-1}]	App. 7
$Elocal_{i,j}$	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. 7
$Eregional_j$	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 PEC_{local} must 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 of this Guidance).

Emission reduction techniques have not been taken into account in the tables of Appendix 7 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. The local PEC 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, the regional PEC is calculated using the annual release rate. It represents the steady-state concentration to be expected, regardless of when the discharge occurred.

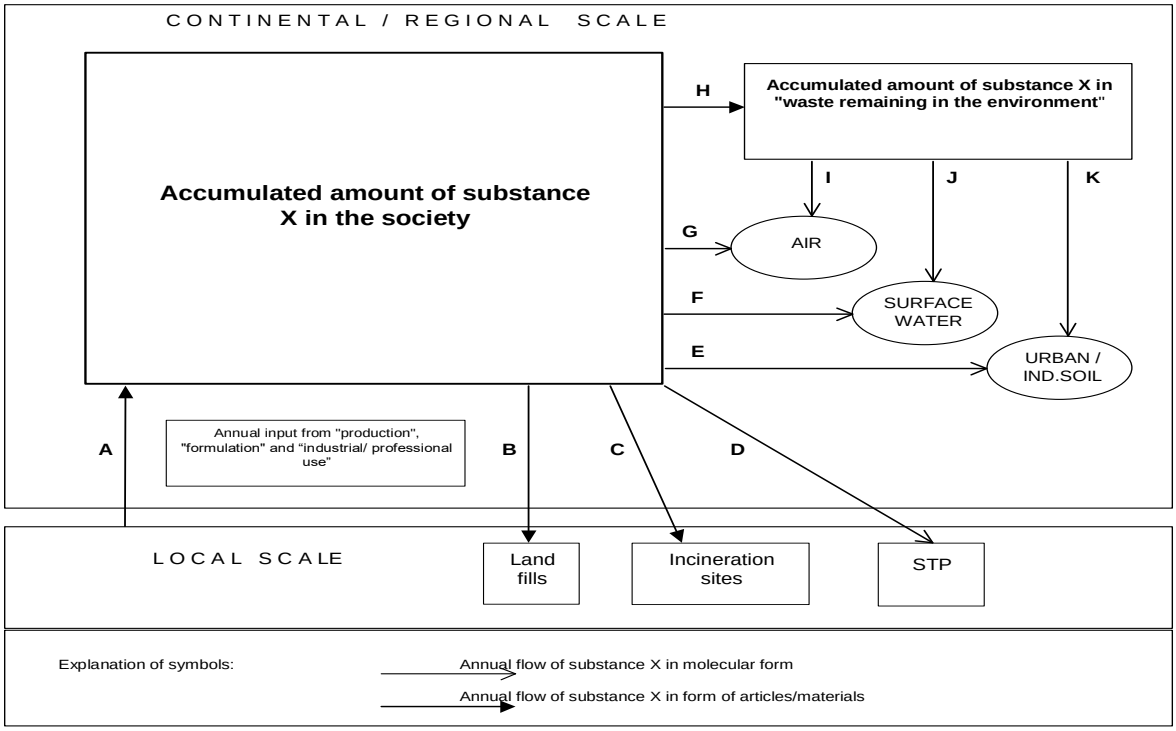
Intermittent release needs to be defined, although applicants and eCAs will have to justify the use of this scenario on a case-by-case basis. Intermittent release can be defined as "intermittent but only recurring infrequently i.e. less than once per month and for no more than 24 hours".

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 local PEC_{water} may also increase the exposure time by repartitioning to the water phase over an extended period. For intermittent releases to the aquatic compartment an intermittent PNEC is used in the risk characterisation (see Section 3.3.2 of this Guidance) 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.



(A = B + C + D + E + F + G + H for society ;
H = I + J + K for "waste remaining in the environment"

Figure 5: Emissions from long-life articles at Steady state

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 emission of biocides from long-life materials, the emission can normally be expected to be highest in the beginning of the use period (due to diffusion mechanisms). It is necessary to be aware that the emission factors are normally an average for the whole service life.

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 scenarios described in ESDs (e.g. ESD PT 8 and the City scenario (PT 10) for (in-can) preservation of paints (PT 6, 7) and polymers (PT 9), ESD PT 2 for in-can preservation of detergents (PT 6), or guidance note on leaching rate estimations of PT 07, 09 and 10)

   - search for data in the literature;

   - use a worst-case assumption or if necessary conduct/request 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 $F_{i,total}$):

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

and:

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

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 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.

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 products or articles at the end of their service life (releases during use and service life 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. 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 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 K_{ow} 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 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 product or article;
- intermediate storage after service life before waste collection;
- 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 2.2.2 of this Guidance). 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 a 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 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 regional PEC (e.g. the sizes of the environmental compartments, mass transfer coefficients) are given in Section 2.3.8.7 (Tables 12-14) of this Guidance.

Table 5: Definition of the standard environmental characteristics

Parameter	Symbol	Unit	Value
General			
Density of the solid phase	RHO_{solid}	$[kg_{solid} \cdot m_{solid}^{-3}]$	2,500
Density of the water phase	RHO_{water}	$[kg_{water} \cdot m_{water}^{-3}]$	1000
Density of air	RHO_{air}	$[kg_{air} \cdot m_{air}^{-3}]$	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			
Bulk density of (wet) suspended matter	RHO_{susp}	$[kg \cdot m^{-3}]$	1,150
Volume fraction solids in susp. matter	$F_{solid, susp}$	$[m_{solid}^{3} \cdot m_{susp}^{-3}]$	0.1
Volume fraction water in susp. matter	$F_{water, susp}$	$[m_{water}^{3} \cdot m_{susp}^{-3}]$	0.9
Weight fraction organic carbon in susp. solids	$F_{oc, susp}$	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.1
Sediment			
Bulk density of (wet) sediment	RHO_{sed}	$[kg \cdot m^{-3}]$	1,300
Volume fraction solids in sediment	$F_{solid, sed}$	$[m_{solid}^{3} \cdot m_{sed}^{-3}]$	0.2
Volume fraction water in sediment	$F_{water, sed}$	$[m_{water}^{3} \cdot m_{sed}^{-3}]$	0.8
Weight fraction organic carbon sediment solids	$F_{oc, sed}$	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.05
Soil			
Bulk density of (wet) soil	RHO_{soil}	$[kg \cdot m^{-3}]$	1,700
Volume fraction solids in soil	$F_{solid, soil}$	$[m_{solid}^{3} \cdot m_{soil}^{-3}]$	0.6
Volume fraction water in soil	$F_{water, soil}$	$[m_{water}^{3} \cdot m_{soil}^{-3}]$	0.2
Volume fraction air in soil	$F_{air, soil}$	$[m_{air}^{3} \cdot m_{soil}^{-3}]$	0.2
Weight fraction organic carbon in soil solids	$F_{oc, soil}$	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.02
Weight fraction organic matter in soil solids	$F_{om, soil}$	$[kg_{om} \cdot kg_{solid}^{-1}]$	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:

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

Application of the formulas above for the values mentioned leads to the following bulk densities of each standard environmental compartment, provided in Table 5 above.

When deriving the bulk density of different environmental compartments care should be taken to ensure that the expression of exposure and effect concentrations is consistent for both (for example always comparing PEC values in dry weight with PNEC values in dry weight or use the corresponding wet weight values for both).

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 of this Guidance. 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. Section 4.5.3 of this Guidance 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.

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

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
$F_{ass,\ aer}$	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; van Noort, 2004):

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

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 (see also *Guidance on information requirements and chemical safety assessment Chapter R.7a: Endpoint specific guidance, Appendix R.7.1-1* Henry's law constant and evaporation rate, (ECHA, 2012c)).

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

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

Explanation of symbols

VP	vapour pressure	[Pa]	data set
MOLW	molecular weight	$[g \cdot mol^{-1}]$	data set
SOL	solubility	$[mg \cdot l^{-1}]$	data set
R	gas constant	$[Pa \cdot m^3 \cdot mol^{-1} \cdot k^{-1}]$	8.314
TEMP	temperature at the air-water interface	[K]	285
HENRY	Henry's law constant	$[Pa \cdot m^3 \cdot mol^{-1}]$	
$K_{air\text{-}water}$	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 are not addressed in this guidance. For further information please refer to *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*.

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:

- K_{oc} measured in a screening test on adsorption/desorption (EC method C.18/OECD Test Guideline 106)
- K_{oc} estimated by the HPLCmethod (EC method C.19/OECD Test Guideline 121);
- column leaching study (OECD 312);
- lysimeter studies/Field leaching studies (OECD Test Guideline 22);

- adsorption control within an inherent biodegradability test;
- if no K_{oc} is available, it may be estimated from K_{ow} "(for metabolites or substances for which a K_{oc} is technically impossible to derive)).

It should be noted that for surfactants the octanol/water partition coefficient (K_{ow}) 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, via standardisation to K_{oc} (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, K_{oc} can be estimated from K_{ow} as outlined in *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*. The equation for "non-hydrophobic" substances is preferred as default. For specific groups of substances, other QSARs are given in *Chapter R.6.* 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 K_{oc} in the assessment. Cationic substances are generally known to adsorb strongly.

For water soluble, highly adsorptive substances the use of K_{ow} 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 K_{ow} (and small Henry's Law constant), while adsorption onto sludge may be a significant elimination mechanism for these substances. For those substances either a K_{oc} experimentally determined *in activated sludge with measured organic carbon content* or the approach described in the following should be used.

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 (K_p) in each compartment (soil, sediment, suspended matter) can be calculated from the K_{oc} 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.

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

Explanation of symbols

K_{oc}	partition coefficient organic carbon-water	[l·kg^{-1}]	data set/Ch. 4
$F_{oc,\ comp}$	weight fraction of organic carbon in compartment *comp*	[kg·kg^{-1}]	Table 5
$K_{p,\ susp}$	partition coefficient solid-water in suspended matter	[l·kg^{-1}]	
$K_{p,\ sed}$	partition coefficient solid-water in sediment	[l·kg^{-1}]	
$K_{p,\ soil}$	partition coefficient solid-water in soil	[l·kg^{-1}]	

K_p is expressed as the concentration of the substance sorbed to solids (in $mg_{chem}·kg_{solid}^{-1}$) divided by the concentration dissolved in porewater ($mg_{chem}·l_{water}^{-1}$). The dimensionless

form of K_p, 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:

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

$$K_{comp\text{-}water} = Fair_{comp} \cdot K_{air\text{-}water} + Fwater_{comp} + Fsolid_{comp} \cdot \frac{Kp_{comp}}{1000} \cdot RHOsolid \quad (24)$$

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

Explanation of symbols

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

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. The rates of degradation of a substance in the environment are determined by a combination of substance-specific properties and environmental conditions.

For substances where a range of degradation data is available, the use of average input parameters (artithmetic mean, median or geometric mean) is recommended.

Please refer also to FOCUS (2006) Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration

(Sanco/10058/2005) and FOCUS (2011), Generic guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration.

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. If relevant metabolites or transformation products are formed, the risk assessment should include these. It is possible that the rate of reaction is such that only the resulting 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 (DT_{50}) of a hydrolysable substance can be converted to degradation rate constants, which may be used in the models for calculating the PEC, if not already covered by results on biodegradation. The results of a ready biodegradability study will show whether or not the hydrolysis products are themselves biodegradable. Similarly, for substances where DT_{50} 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 *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*.

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:

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

where X = 12 °C for fresh water and 9 °C for seawater. 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:

$$khydr_{water} = \frac{\ln 2}{DT50\,hydr_{water}} \quad (26)$$

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 regional PEC 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:

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

Explanation of symbols

$DT_{50}photo_{water}$	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 like AOPWIN (US EPA, 2012).

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
$OHCONC_{air}$	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. 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 (e.g. OECD Test guideline 303 A). For further guidance on use of STP simulation test results, see Section 2.3.7 of this Guidance.

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.

If measured degradation rates for the STP are available, no temperature correction is needed for these rates.

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 on Table 6:

a) Ready biodegradability testing (28 d) e.g. according to OECD test guidelines 301 A-F. 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. If appropriate, re-testing in another more suitable ready biodegradability 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) e.g. according to OECD test guidelines 302 B-C.

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 should be conducted (OECD test guideline 303 A).

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, and 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 (OECD test guideline 302 A). 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 and concentration 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.

In some circumstance specific information on biodegradability in water, sediment or soil may not be available. However any deviations from the core and PT-specific information requirements (see *Guidance on the BPR: Volume IV Environment, Part A Information Requirements*) should be clearly justified. In these cases it may be justifiable that 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.

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.

Surface water

Use of simulation test results:

Preference of simulation tests (e.g. OECD Test guideline 309) also applies to estimation of degradation half-life in surface waters. 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.

Use of screening test results:

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 not affect the local concentration but only 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 on 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 as well as a solid phase and soil containing air, porewater as well as 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.

Soil and sediment:

Use of simulation test results:

Also for assessment of biodegradation in soil or sediment, data from relevant simulation tests (e.g. OECD Test guideline 307 and 308) are preferred. Of course these tests do 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. However if up to three DT_{50}-values from different water-sediment or soil systems are available, the worst case value will be used whereas when more than three DT_{50}-values for the respective compartment are available then the geometric mean will be used.

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. For field degradation/dissipation studies, where the compound might be lost not only because of actual degradation but also because of photolysis, volatilization, leaching or surface runoff, the significance of loss due to transport should be estimated based on known compound properties (e.g. Henry's law constant, solubility or the K_{ow}). If considerable losses to other compartments cannot be excluded, preference should be given to degradation data obtained under controlled laboratory conditions for the evaluation of the substance´s persistence. Another possible approach for soil is that in case of a biphasic decline only the slow phase of this decline should be taken into account into account for estimating the half-life since this reflects the degradation in the soil matrix rather than loss-processes at the soil surface.

Use of screening test results:

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 K_p 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 K_p values there is evidence that some sort of K_p dependence exists. Therefore degradation half-life classes for (bulk) soil, partly based on K_p 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 $K_{p, soil}$ values are preferred, but if not available and assuming an EU standard soil these values correspond to log K_{ow} values of 4.4 ($K_{p, soil}$ = 100), 5.7 ($K_{p, soil}$ = 1000), and 6.9 ($K_{p, soil}$ = 10,000) using the TGD QSAR equations for $K_{p, soil}$ as a function of K_{ow}

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). However, this has to be considered on a case-by-case basis. The following equation can be used to convert DT_{50} to a rate constant for biodegradation in soil:

$$kbio_{soil} = \frac{\ln 2}{DT50\,bio_{soil}} \quad (29)$$

Explanation of symbols

$DT_{50}bio_{soil}$	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:

$$kbio_{sed} = \frac{\ln 2}{DT50 bio_{soil}} \cdot Faer_{sed} \quad (30)$$

Explanation of symbols

$DT_{50,\,bio,\,soil}$	half-life for biodegradation in bulk soil	[d]	Table 8
$F_{aer,\,sed}$	fraction of the sediment compartment that is aerobic	[$m^3 \cdot m^{-3}$]	0.10
$k_{bio,\,sed}$	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 regional PEC, 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 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}]	

2.3.7.1. Wastewater treatment

In this section, the following parameters are derived:

- emission from a sewage treatment plant 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 4). The percentage connection rate across the Community is subject to improvement due to the implementation of Council Directive 91/271/EEC of 21 May 1991 concerning 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. A figure of 90% connection to wastewater treatment is proposed for the regional standard environment (see Appendix 4). 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 of this Guidance) it is assumed that 90% of the wastewater is treated in a biological STP and the remaining 10% 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 by using EUSES or Simple Treat.

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 sewage treatment plant or other environmental situations, for example a river (see Volume IV, Part A).

There is insufficient information available on the applicability of elimination data from the laboratory test to the processes of a real sewage treatment 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 using EUSES or Simple Treat.

Infobox 3: EUSES

EUSES is a decision-support tool which enables the user to calculate the risk for the environment. The TGD (2003) as well as finalised emission scenario documents for biocides are included in EUSES 2.1.2

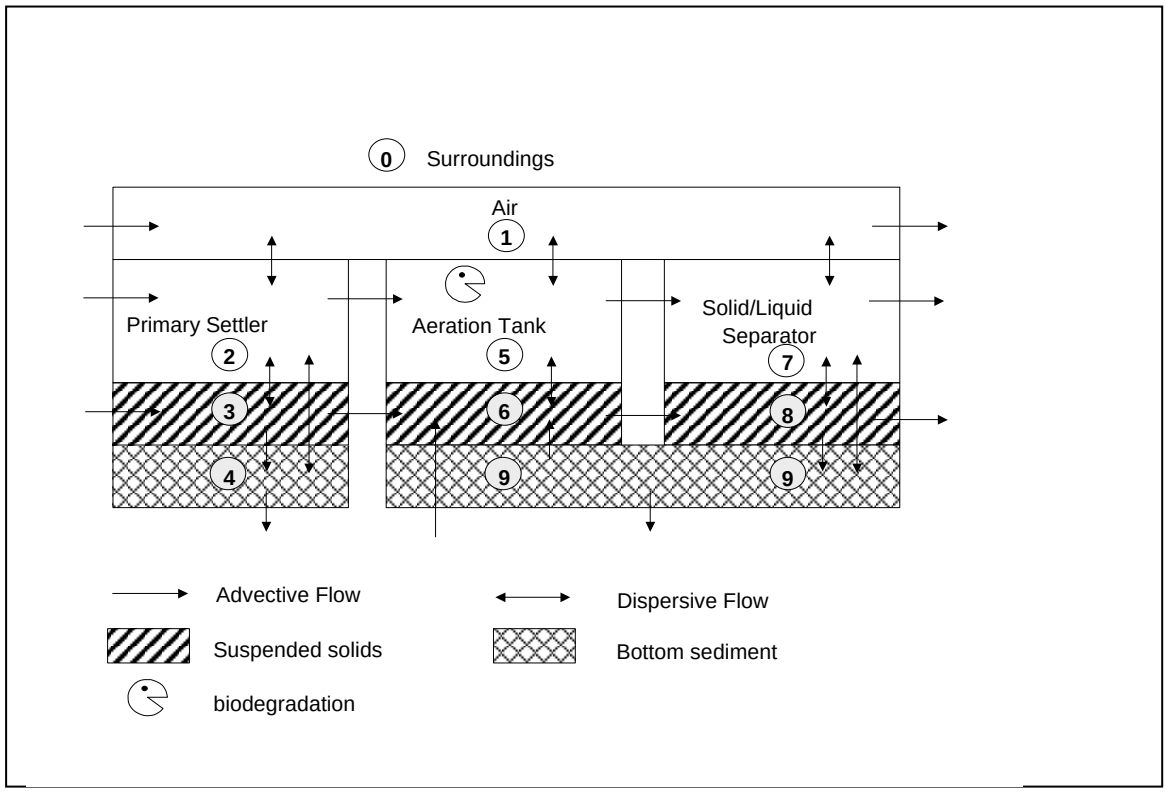
EUSES (2.1.2) and a manual to the program can freely be downloaded from the internet (http://ihcp.jrc.ec.europa.eu/our_activities/public-health/risk_assessment_of_Biocides/euses) and can be run on a normal PC. EUSES can be used for the environmental exposure estimation with the release estimation from Section 2.3.3.3 of this Guidance. Besides the release estimation, only a few data on substance properties are needed to calculate PECs. If the use of default exposure estimates do not lead to a conclusion of safe use, a refined assessment is possible for example by including more specific information on releases and improved data on substance properties.

Output: The output of EUSES consists of the predicted environmental concentrations (PECs) for environmental risk assessment. EUSES can prepare an electronic report of all the input and output data in a Word or Excel format.

Modelling STP

If there are no measured data available, the degree of removal can be estimated by means of a sewage treatment plant model using log K_{ow} (K_{oc} or more specific partition coefficients can also be used; see Section 2.3.5 of this Guidance), 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.

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).

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

* including rainwater

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.

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

Explanation of symbols

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

Calculation of the STP-effluent concentration

The concentration of the effluent of the STP is given by the fraction directed to effluent and the concentration in untreated wastewater as follows:

$$Clocal_{eff} = Clocal_{inf} \cdot Fstp_{water} \quad (33)$$

Explanation of symbols

$Clocal_{inf}$	concentration in untreated wastewater	[mg·l^{-1}]	eq. (32)
$Fstp_{water}$	fraction of emission directed to water by STP	[-]	Estimation by EUSES/Simple Treat
$Clocal_{eff}$	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]	10000 (see Table 9)
WASTEWinhab	sewage flow per inhabitant	[l·d^{-1}·eq^{-1}]	200 (see Table 9)
$EFFLUENT_{stp}$	effluent discharge rate of STP	[l·d^{-1}]	2 x 10^6

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

Infobox 4: Recommended method to calculate the concentration in the STP effluent

The EUSES/Simple Treat method should be used for calculating the fate and behaviour of a substance in the STP instead of the formerly used tables in Appendix II of TGD (2003).

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

$F_{stp,\ air}$	fraction of the emission to air from STP	[-]	Estimation by EUSES/Simple treat
$Elocal_{water}$	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	[-]	Estimation by EUSES/Simple treat
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:

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

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:

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

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 of this Guidance 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·l^{-1}]	eq. (32)
PEC_{stp}	PEC for microorganisms in the STP	[mg·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 sewage 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.

2.3.8. Calculation of PECs

In this section, the local PECs for all environmental compartments are derived.

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 of this Guidance, the calculation of regional steady-state concentrations ($PEC_{regional}$) 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 ($PEC_{local,\ water}$) is in principle calculated after complete mixing of the effluent. 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 of this Guidance). 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 ($PEC_{local,soil}$) 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 of this Guidance) (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 (see Table 11). 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 ($PEC_{local,\ air}$) 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 of this Guidance). 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 of this Guidance). Emissions are assumed to be a continuous and diffuse flux into the environment.

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 exposure assessment of the marine environment is presented in Section 2.6 of this Guidance.

Figure 7 Local relevant emission and distribution routes

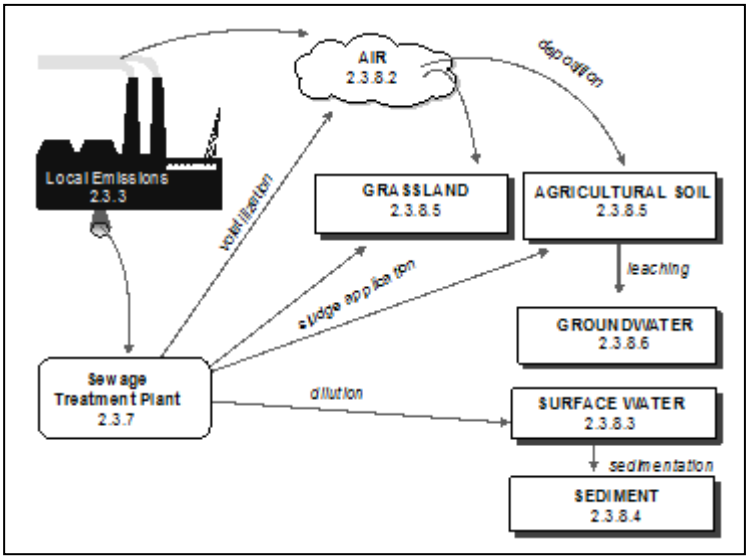


Figure 7 shows the relationship between the local emission routes and the subsequent distribution processes, which may be relevant for the different environmental compartments. For each compartment, specific fate and distribution models are applied.

Table 10: Overview of different exposure scenarios and the respective PECs

Target	Medium of exposure	Exposure scenario				
		regional	Section	local		Section
Aquatic compartment	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 PEC_{local} 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.

PEC_{local} for air cannot be compared with the PNEC for air because the latter is usually not available. The PEC_{local} 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 PEC_{local} in soil. Therefore, both deposition flux and concentration are calculated as annual average values.

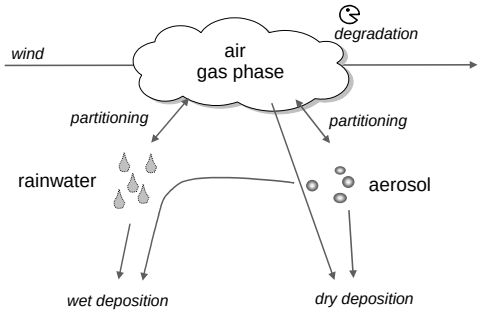


Figure 8: Fate processes in the air compartment

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 active substances or substances of concern, 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 estimated by using AOPWIN (US EPA, 2012). Please refer also to paragraph 2.3.6.3 when calculating the atmospheric reaction rate.
- 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 PEC_{local} 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 ($PEC_{regional}$) is used as background concentration if the exposure assessment is performed using the tonnage based approach 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 PEC_{local}:

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

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

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)
$PEC_{regional,air}$	regional concentration in air	[mg·m^{-3}]	2.3.8.7
$PEC_{local, air,ann}$	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)
$F_{ass, aer}$	fraction of the substance bound to aerosol	[-]	eq. (19)
$DEP_{std, aer}$	standard deposition flux of aerosol-bound compounds at a source strength of 1 kg·d^{-1}	[mg·m^{-2}·d^{-1}]	1·10^{-2}
$DEP_{std, gas}$	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
DEP_{total}	total deposition flux during emission episode	[mg·m^{-2}.d^{-1}]	
$DEP_{total, ann}$	annual average total deposition flux	[mg.m^{-2}.d^{-1}]	

2.3.8.3. Calculation of PEC_{local} for the aquatic compartment

In this section, the local concentration in surface water during emission episode is derived. It can be distinguished between indirect release to surface water, when another environmental compartment (e.g. STP) is exposed before or direct release, when surface water is the first receiving environmental compartment.

Indirect release:

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.

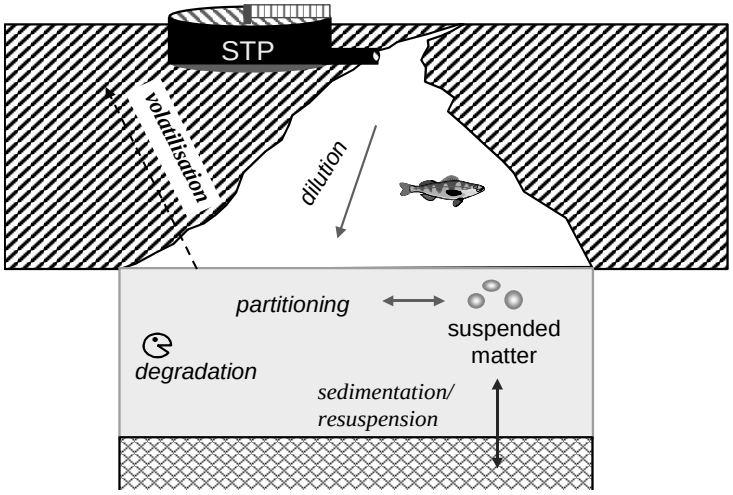


Figure 9: Fate processes in surface water

The calculation of the PEC_{local} 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 depends on the dimensions of the STP and the receiving surface water and on the flow rate of effluent discharge of the STP in relation to the flow rate of the receiving surface water. 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, like e.g. preservatives in polymerised materials – see Section 2.3.3.5 of this Guidance) 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, $K_{p,\ susp}$, it can be estimated from the K_{oc} of the substance, determined for other sorbents like soil or sediments (Section 2.3.5 of this Guidance) 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 exceed the water solubility of the substance. 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 addresses the specific emission pattern as well as river parameters.

The local concentration in surface water is calculated as follows.

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

Explanation of symbols

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

When considering dilution factors, account should be taken of the fluctuating flow-rates of typical receiving waters. The low-flow rate (or 10th 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):

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}} \quad (46)$$

Explanation of symbols

$EFFLUENT_{stp}$	effluent discharge rate of stp	[l·d^{-1}]	eq. (34)
FLOW	flow rate of the river	[l·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:

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365} \quad (47)$$

Explanation of symbols

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

The concentration at the regional scale ($PEC_{regional,\ water}$) is used as background concentration for the local scale if the exposure assessment is performed using the tonnage based approach. Therefore, these concentrations are summed:

$$PEClocal_{water} = Clocal_{water} + PECregional_{water} \quad (48)$$

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECregional_{water} \quad (49)$$

Explanation of symbols

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

Direct release:

In the following product-types, passing an STP is not an option but direct emission to surface water (fresh water or seawater) occurs:

PT 2: Swimming pools

PT 4: Seawater desalination

PT 6: Preservatives for product during storage

PT 7: Film preservatives

PT 8: Wood preservatives (use classes 3: bridge over pond, 4b: jetty in a lake/sheet piling in a waterway and 5: harbour wharf)

PT 9: Specifically fiber, rubber and polymerised materials preservatives

PT 11: Preservatives for liquid cooling and processing systems (e.g. "once through" cooling systems)

PT 12: Paper and wood pulp/Oil extraction

PT 17 Piscicides

PT 18: Control of mosquito larvae

PT 19: Repellents and attractants

PT 21: Antifouling products

For these cases specific guidance on how to perform the exposure assessment for surface water is provided in the respective ESD (see Table 4). Please not that PT 6, PT 7, PT 9 and PT 10 are covered with regard to exposure assessment of surface water by the ESD for PT 8.

2.3.8.4. Calculation of PEC_{local} for sediment

In this section, the following parameter is derived:

- local concentration in sediment during the emission episode.

PEC_{local} 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

$PEC_{local,\ water}$	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)
$PEC_{local,\ sed}$	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 of this Guidance) 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 PEC_{local} for the soil compartment

The PEC in agricultural soil is used for risk characterisation of terrestrial ecosystems (Section 4 of this Guidance) and as a starting point for the calculation of indirect human exposure via crops and cattle products (see BPR Volume III Human health, Part B Risk Assessment).

The following Figure 10 shows the most important fate processes in the soil compartment.

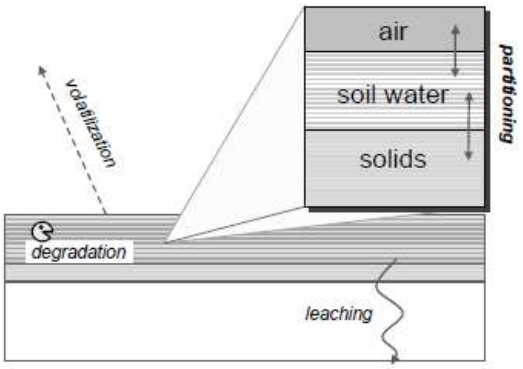


Figure 10: Fate processes in the soil compartment

It can be distinguished between indirect releases to soil, when another environmental compartment is exposed before (e.g. release via sewage sludge application from a STP) or direct release, when soil is the first receiving environmental compartment.

Indirect release:

In this section, the following endpoints and underlaying 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).

Guidance for calculating PEC_{local} in soil is given for the following exposure routes:

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

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. 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. **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. 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 of this Guidance) and is related to a surrounding area within 1000 m from that source. The deposition is averaged over the whole area.

For the exposure assessment of soil, 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.

Initial concentration:

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

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

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:

$$D_{air} = \frac{DEPtotal_{ann}}{DEPTH_{soil} \cdot RHO_{soil}} \quad (52)$$

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:

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

C_{soil} (0)	initial concentration in soil after sludge application	[mg·kg^{-1}]	eq (51)
C_{soil} (t)	concentration in soil at a specific moment in time after sludge application	[mg·kg^{-1}]	

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

Average concentration:

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.

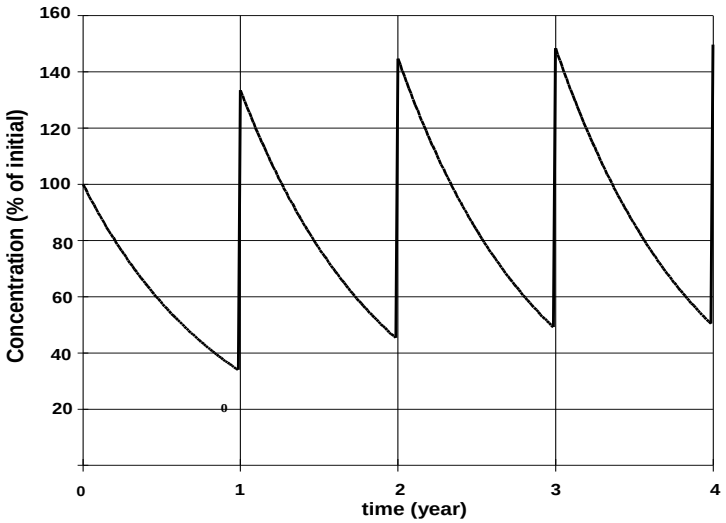


Figure 11: Cumulation in soil due to several years of sludge application

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.

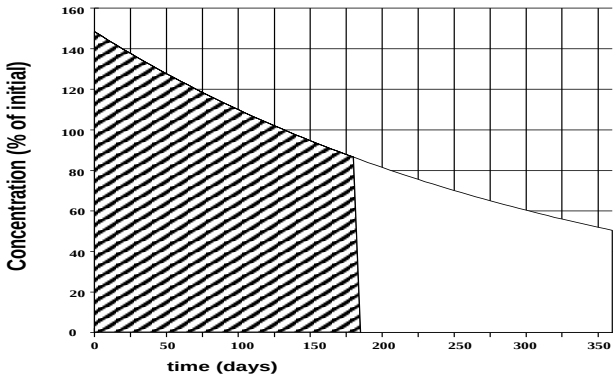


Figure 12: The concentration in soil after 10 years. The shaded area is the integrated concentration over a period of 180 days

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:

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

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)
$C_{local, soil}$	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 (please refer to section 2.3.6.5 of this Guidance);
- 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.
Given a substance-independent air-side partial mass transfer coefficient, $kasl_{air}$, the soil-referenced overall mass transfer coefficient, used for calculating the rate constant for volatilization, $k_{volat\,i}$, becomes:

$$\frac{1}{k_{volat\,i}} = \left(\frac{1}{kasl_{air} \cdot K_{air\text{-}water} / K_{soil-water}} + \frac{1}{kasl_{soil}} \right) \cdot DEPTH_i \qquad (57)$$

,where $K_{air-soil}$, $K_{air-water}$ and $K_{soil-water}$ are the dimensionless equilibrium constants between bulk air and bulk soil, bulk air and bulk water, and between bulk soil and bulk water, respectively, and DEPTHi (m) is the mixing depth of the soil compartment.

Explanation of symbols

$kasl_{air}$	partial mass transfer coeff. at air-side of the air-soil interface	[m·d^{-1}]	120
$kasl_{soilair}$	partial mass transfer coeff. at soilair-side of the air-soil int.	[m·d^{-1}]	0.48
$K_{air-water}$	air-water partitioning coefficient	[m^3·m^{-3}]	eq. (22)
$K_{soil-water}$	soil-water partitioning coefficient	[m^3·m^{-3}]	eq. (24)
$DEPTH_i$	mixing depth of soil type *i*	[m]	Table 11
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	[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:

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

Explanation of symbols

$F_{inf,\ soil}$	fraction of rain water that infiltrates into soil	[-]	0.25
RAINrate	rate of wet precipitation (700 mm/year)	[m.d^{-1}]	$1.92 \cdot 10^{-3}$
$K_{soil-water}$	soil-water partitioning coefficient	[m^3·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:

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

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:

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

Explanation of symbols

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

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

$$Facc = e^{-365\ k} \quad (61)$$

Explanation of symbols

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

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

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

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

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

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:

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

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)
$F_{st\text{-}st}$	fraction of steady-state in soil achieved	[-]	

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

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

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)
F_{acc}	fraction accumulation in one year	[-]	eq. (61)
$C_{sludge,\ soil\ 1}(0)$	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 $PEC_{local,\ soil}$

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	Averaging time	Rate of sludge application	Endpoint
	[m]	[days]	[kgdwt.m-2.year-1]	
$PEC_{local,soil}$	0.20	30	0.5	terrestrial ecosystem
$PEC_{local,\ agr.\ soil}$	0.20	180	0.5	crops for human consumption
$PEC_{local,\ grassland}$	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 are 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 if the exposure assessment is performed using the tonnage based approach. 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

$C_{local,\ soil}$	local concentration in soil	[mg·kg^{-1}]	eq. (54)
$PEC_{regional,\ natural\ soil}$	regional concentration in natural soil	[mg·kg^{-1}]	2.3.8.7
$PEC_{local,\ soil}$	predicted environmental conc. in soil	[mg·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

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

Direct release:

In the following product-types, substances can potentially be directly released to soil without passing an STP or any other environmental compartment before:

PT 6: Preservatives for product during storage

PT 7: Film preservatives

PT 8: Wood preservatives (use classes 3, 4b and 5)

PT 9: Fibre, leather, rubber and polymerised materials preservatives

PT 10: Construction material preservatives

PT14: Rodenticides

PT18: Insecticides, acaricides and products to control other arthropods

For these cases specific guidance on how to perform the exposure assessment for soil is provided in the respective ESD (see Table 4). Please not that PT 6, PT 7, PT 9 and PT 10 are coverd with regard to exposure assessment of soil by the ESD for PT 8.

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. 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

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

As refinement option, the $PEC_{local,gw}$ can be estimated by using available groundwater simulation models developed for assessment of the pesticide mobility in soil reflecting, more realistic groundwater conditions, or by using measured data (lysimeter studies or monitoring data).

Available groundwater simulation models are PEARL or PELMO which make use of harmonized European standard scenarios for soil and environmental characteristics. For active substance approval PEARL has been selected as the preferably model to be used. All nine available scenarios in PEARL should be run and the outcome should be reported. However, for substance approval, only one scenario needs to meet the required criteria according to the BPR Annex VI, point 68. A full description of these models can be found

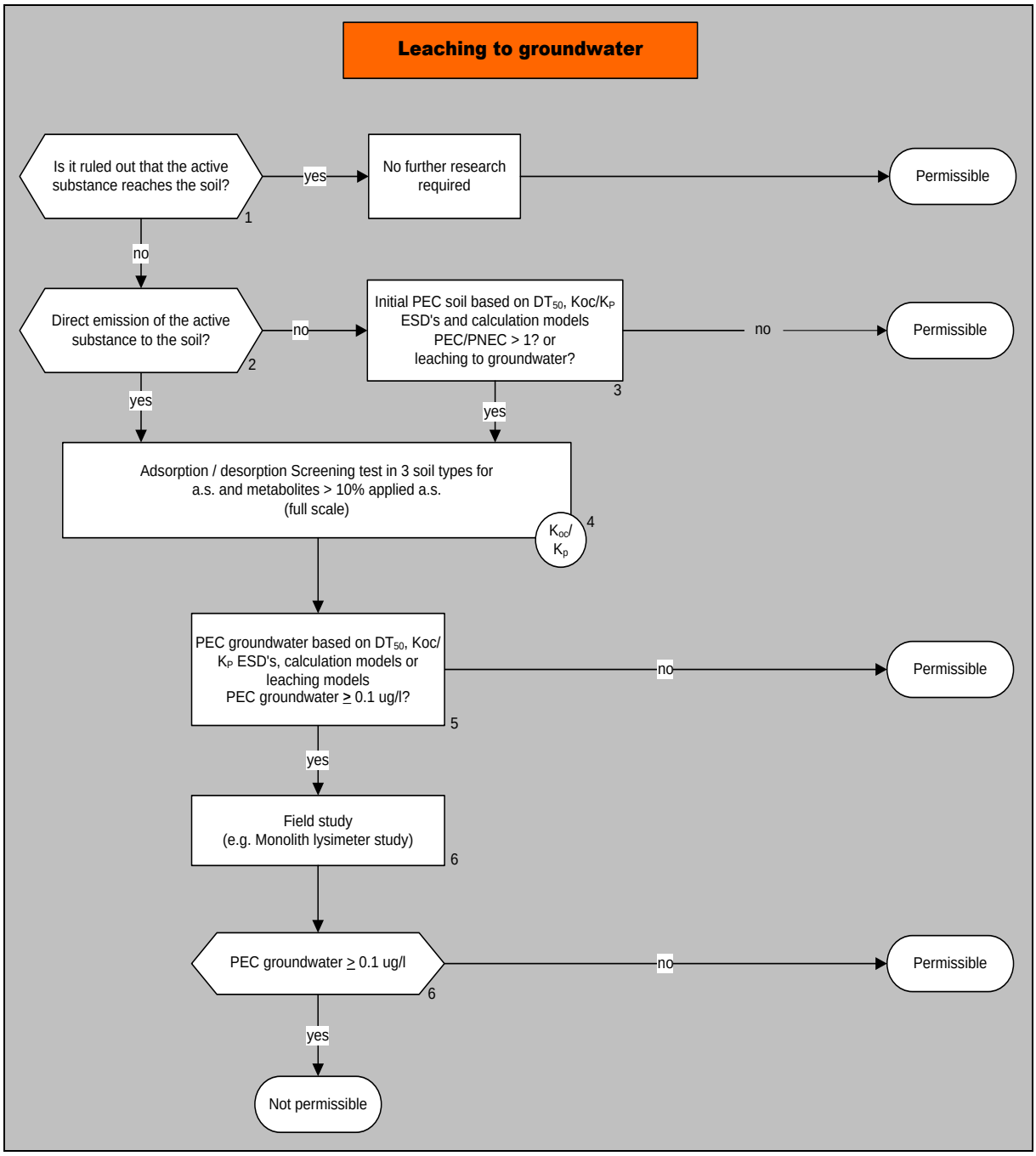
in: FOCUS groundwater scenarios in the EU review of active substances or Generic guidance for FOCUS groundwater scenarios.

Lysimeter studies and monitoring data need to be assessed case by case. For lysimeter studies, some technical guidance can be found in "Guidance to interpretation of field and lysimeter studies can be found in Verschoor et al. (2001) - http://www.rivm.nl/bibliotheek/rapporten/601506007.html.

Groundwater criteria evaluation summary

The BPR implies that for biocides the trigger value for pesticides in groundwater is applied (BPR Annex VI, point 68). The concentration in groundwater should therefore be <0.1 µg/L for active substance, relevant metabolites or breakdown/reaction products and substances of concern. The total concentration should be <0.5 µg/L. In addition, the trigger value applies for each separate biocide. A decision tree is given in Figure 13:

Figure 13: Decision tree for the groundwater assessment



2.3.8.7. Calculation of $PEC_{regional}$

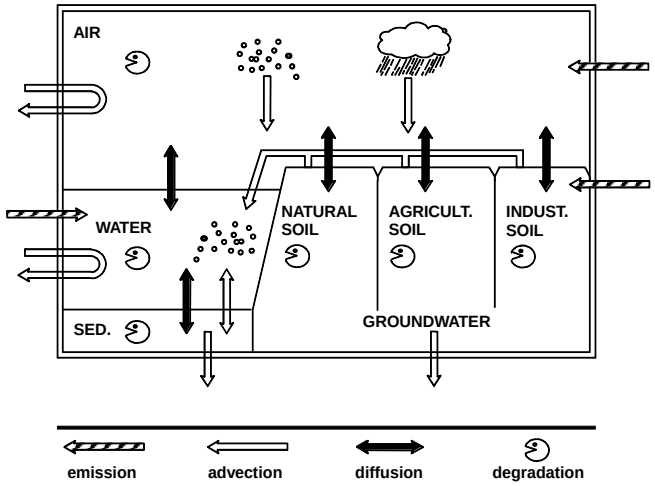
In this section, the following parameters are derived:

- 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 7) 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 14:

Figure 14: 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 $PEC_{regional}$ calculation, in contrast to PEC_{local}, 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 90% (the EU average according to Appendix 4) 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 $PEC_{regional}$

When calculating the $PEC_{regional}$ 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 $PEC_{regional}$ on the basis of a standardised regional environment with agreed model parameters;
- calculation of a $PEC_{regional}$ on the basis of country specific model parameters.

A standardised regional environment should be used for the first approach in the calculation of $PEC_{regional}$. 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·s^{-1}
air-water interface: water side partial mass transfer coefficient	$1.39 \cdot 10^{-5}$ m·s^{-1}
Aerosol deposition rate	0.001 m·s^{-1}
air-soil interface: air side partial mass transfer coefficient	$1.39 \cdot 10^{-3}$ m·s^{-1}
air-soil interface: soilair side partial mass transfer coefficient	$5.56 \cdot 10^{-6}$ m·s^{-1}
air-soil interface: soilwater side partial mass transfer coefficient	$5.56 \cdot 10^{-10}$ m·s^{-1}
sediment-water interface: water side partial mass transfer coefficient	$2.78 \cdot 10^{-6}$ m·s^{-1}
sediment-water interface: pore water side partial mass transfer coefficient	$2.78 \cdot 10^{-8}$ m·s^{-1}
net sedimentation rate	3 mm·yr^{-1}

Model parameters for the continental concentration

The continental box covers 15 EU countries and Norway and similar percentages for water and natural, agricultural and industrial/urban soils as given in Table 13. 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

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

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

2.4. Use of measured data

For a number of existing active substances measured data are available for air, fresh- or seawater, 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 of this Guidance);
- 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 of this Guidance);
- 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 of this Guidance).

2.4.1. Selection of adequate measured data

The available measurements have to be assessed first, before using them in release and exposure estimation. The following aspects should be considered:

- Quality of the sampling and analytical techniques
- Selection of representative data for the environmental compartment of concern
- Outliers
- Treatment of values below the limit of quantification (LOQ)
- Data comparability

Applicants and evaluating authorities should also consider local regulatory requirements where applicable. Local agencies may have specific requirements on how data should be statistically analysed. It is advisable to obtain as much useful information on release and 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, based on the available contextual information, are given in Table 15 below (based on OECD, 2000). 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 and the availability of information necessary to assess the representativeness of the sample.

Table 15: 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 on Table 15:

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.

Quality of the sampling and analytical 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 quantification (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).

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

The representativeness of the monitoring data is related to the objective of the monitoring programme from which they originate. Monitoring programmes may be designed to cover a large spatial area (high number of stations over a large territory), to achieve a high spatial resolution (high number of stations per area unit), or to monitor only one point source release. Monitoring programmes may be designed to assess temporal trends (high sampling frequency), or to monitor the status of a site at a given time.

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 and would not be appropriate for a local assessment.

For example, when evaluating the representativeness of discharges from a wastewater treatment plant, the number of samples and the sampling frequency should be adapted *inter alia* to the type of treatment process (including retention time), environmental significance and nature of the substance and effluent variability. Effluent quality and quantity vary over time in terms of volumes discharged and constituent concentrations. Variations occur due to a number of factors, including changes in human activity, changes in production cycles, variation performance of wastewater treatment systems in particular in responses to influent changes and changes in climate. Even in industries that operate continuous processes, maintenance operations, such as back-washing of filters, cause peaks in effluent constituent concentrations and volumes (US-EPA, 1991).

Data from a prolonged monitoring programme, where seasonal fluctuations are already included, are of special interest. However, too old data may not be representative of the risk management measures and operating conditions described in the exposure scenario. Indeed, pollution may have been reduced or increased by the implementation of risk management measures or of operation conditions, by new releases or change in release pattern.

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 90^{th} percentile values, mean or median values of this distribution could be used in the PEC prediction. The mean of the 90^{th} 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. A 90^{th} percentile concentration may also be calculated. In most instances a log-normal distribution of concentrations can be assumed. 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 release episodes of short duration but of high concentration discharge. In these cases, mainly for PEC_{local} calculations, a more realistic picture of the release pattern can be obtained from the highest value of average concentrations during release episodes.

When considering data about dilution, it should be taken into account that flow rates of receiving waters are typically highly fluctuating. In this case, the 10^{th} percentile, corresponding to the low flow rate, should always be used. If only time averaged flow rates are available, the flow rate for dilution purposes should be estimated as one third of the average.

When releases 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 to obtain flow-weighted concentrations. As a surrogate and complement, average time trend data on real runoff or landfill gas production data can also be used to extend flux measures to long-term estimates. Release data of higher quality may be available in the European Pollutant Release and Transfer Register (E-PRTR)[9].

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 time lags. 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 a non-steady-state. Representative and reliable measured data from monitoring programmes or from literature should be compiled as tables and annexed to the risk assessment report. The measured data should be presented with the relevant contextual information in the following manner:

Table 16: Table for presenting data

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

Concentrations can be measured in the receiving environment or in the release. If the reported concentration has been measured directly in the release, this should be clearly indicated in the reporting table.

Outliers

Outliers can be defined as unexpectedly high or low values. Outliers may reflect:

- sampling or analytical flaws;
- other errors (e.g. in data capture or treatment);
- random variability;

9 http://prtr.ec.europa.eu/

- accidental, increased or new release, a recent change in release pattern or a newly discovered occurrence in a specific environmental compartment.

Sampling or analytical errors could potentially be demonstrated after quality check of the sampling and analytical methodologies (see previous section). Data with evident mistakes (e.g. wrong units, errors in data capture, etc.) should be discarded or corrected. Measured concentrations caused by an accidental release should not be considered in the exposure estimation.

Outliers are, by definition, infrequent and implausible measurements, i.e. unlikely to be explained by the random variability of the data alone. The probability of deviation of a measurement from the rest of the measurements due to random variability of the data can be quantified assuming a statistical distribution of the data (e.g. using the Grubbs' test (Grubbs, 1969)). But simpler empirical criteria may also be applied to detect outliers[10] (EC, 1999; USEPA (2006)).

Where outliers have been identified their inclusion/exclusion should be discussed and justified. The data should be critically examined with regard to the possible explanations listed above. Extreme values may reflect an actual sudden increase of releases, discharges or losses of the substance, and this should of course be considered in the assessment.

Treatment of measurements below the limit of quantification

A commonly encountered problem when working with monitoring data is the use of concentrations below the LOQ of the analytical method. At very low concentration levels, random fluctuations become preponderant and the uncertainty of the measurement is significantly high. Clearly at concentrations approaching the LOQ of an analytical method, percentage errors will be greater than at higher concentrations.

All measurements below the LOQ constitute a special problem and should be considered on a case-by-case basis. It should be checked first that the matrix analysed is the most appropriate (e.g. hydrophobic substances should be analysed in sediment or biota rather than in water) and that the analytical technique being used is suitable and sensitive enough (EC, 2009a). In the absence of adequate method of analysis for the substance or in case of substances that are toxic in extremely low concentrations, one approach that could be considered would be to use a value corresponding to LOQ/2 (EC, 2009b). As this method could heavily influence the assessment (e.g. when calculating a mean or a standard deviation), other methods may also be considered (e.g. assuming same distribution of data below and above the LOQ) (EC, 1999).

Data comparability

Another important point to check is the comparability of the data. 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).

Samples of living organisms (= biota) 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 a release source or on a regional scale. Furthermore they can provide a PEC_{biota} and consequently an estimation

[10] For example the following approach may be used: $log(X_i) > log(p_{75}) + K(log(p_{75}) - log(p_{25}))$
Where X_i is the concentration, above which a measured value may be considered an outlier, pi is the value of the ith 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.

of the body burden to be considered in the food chain. But concentrations in biota can vary depending on species (mainly because of different feeding habits and different metabolic pathways) and on other factors such as age, size, lipid content, sex, season etc. These pieces of information should be considered carefully before comparing or aggregating measured concentrations in biota. For instance, normalisation for the lipid content is a common practice when working with monitoring data in biota. Please refer also to the specific guidance on chemical monitoring of sediment and biota for the implementation of Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy (the "Water Framework Directive").

2.4.2. Allocation of the measured data to a local or regional scale

Concentrations measured in the receiving environment should be allocated to a local or regional scale in order to define the nature of the environmental concentration that is derived. If there is no spatial proximity between the sampling site and point sources of release (e.g. from rural regions), the data represent a regional concentration ($PEC_{regional}$) that has to be added to the calculated PEC_{local}. If the measured concentrations reflect the releases into the environment through point sources, they are of a PEC_{local}-type. In a PEC_{local} based on measured concentrations, the regional concentration (i.e. $PEC_{regional}$) is by definition already included.

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. 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 $PEC_{regional}$ 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 must 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.

2.6. Marine exposure assessment

2.6.1. Introduction

While the approaches to the exposure assessment for the marine compartment must be conform to EC requirements for assessment under the Directive 67/548, the REACH Regulation and the BPR, 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 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 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 above, the concern stated under "a" 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 PBT, 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.

2.6.2. Measured data

Guidance on the use of measured data in inland environment also applies to the marine environment. Please refer to Section 2.4 of this Guidance.

2.6.3. Partition coefficients

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 of this Guidance. 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 of this Guidance. 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 K_{ow} dependency of the pH directly (cf. the new draft OECD guideline 122 "Log K_{ow} 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 Section 4.5.3 of this Guidance, 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.

2.6.4. Marine degradation

2.6.4.1. 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.

2.6.4.2. 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.

2.6.4.3. 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 must 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 (OECD 309 or OECD 308) by using samples from the particular environment as inoculum. Nevertheless, data from anaerobic screening tests conducted with digested sewage sludge cannot be used for predicting the degradation potential in sediments.

2.6.4.4. Use of biodegradation screening test data

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 17.

Table 17: 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	∞	∞	∞

n.a. = not applicable

Notes on Table 17:

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. The half-life of 150 days is not fully scientifically justifiable, 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 only added for the sake of completeness, they are only to be used in case a regional assessment (coastal model) is conducted as described in Section 2.6.6 of this Guidance.

The half-lives for the marine environments that are described in Table 17 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 17).

2.6.5. Local Assessment

2.6.5.1. 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.

2.6.5.2. Calculation of PEC_{local} 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 PEC_{local} 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 ($C_{local, seawater}$).

Regarding the presence or absence of a STP, conflicting information is available. Experience with the risk assessment of 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 7), 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 of this Guidance).

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 ($C_{local,\ seawater}$, see Section 2.3.8.3, equations 45-49 of this Guidance).

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

$C_{local,\ eff}$	concentration of the substance in the STP effluent	[mg·l^{-1}]	eq. (33)
$K_{p,\ susp}$	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
$C_{local,\ seawater}$	local concentration in seawater during emission episode	[mg·l^{-1}]	

$K_{p,\ susp}$ is derived as for inland risk assessment. For a specific estimation of the partitioning behaviour of substances in seawater environments see Section 2.6.3 of this Guidance.

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 i.e. 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 seawater is calculated:

$$Clocal_{seawater,ann} = Clocal_{seawater} \cdot \frac{Temission}{365} \quad (84)$$

Explanation of symbols

$C_{local,\ seawater}$	local concentration in seawater during emission episode	[mg·l^{-1}]	eq. (83)
$T_{emission}$	number of days per year that the emission takes place	[d·yr^{-1}]	App. IB
$C_{local,\ seawater,ann}$	annual average local concentration in seawater	[mg·l^{-1}]	

The concentration at the regional scale ($PEC_{regional,seawater}$) is used as background concentration for the local scale, if the exposure assessment is preformed using the tonnage based approach. Therefore, these concentrations are summed:

$$PEClocal_{seawater} = Clocal_{seawater} + PECregional_{seawater} \quad (85)$$

$$PEClocal_{seawater,ann} = Clocal_{seawater,ann} + PECregional_{seawater} \quad (86)$$

Explanation of symbols

$C_{local,\ seawater}$	local concentration in seawater during episode	[mg·l^{-1}]	eq. (83)
$C_{local,\ seawater,ann}$	annual average concentration in seawater	[mg·l^{-1}]	eq. (84)
$PEC_{regional,seawater}$	regional concentration in seawater	[mg·l^{-1}]	4.2.5
$PEC_{local,seawater}$	predicted environmental concentration during episode	[mg·l^{-1}]	
$PEC_{local,seawater,ann}$	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[11];
- 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.

2.6.5.3. Calculation of PEC_{local} for the sediment compartment

[11] 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.

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):

$$PEClocal_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PEClocal_{seawater} \cdot 1000 \quad (87)$$

Explanation of symbols

$PEC_{local, seawater}$	concentration in seawater during emission episode	[mg·l^{-1}]	
$K_{susp-water}$	suspended matter-water partitioning coefficient	[m^3·m^{-3}]	eq. (24)
RHO_{susp}	bulk density of suspended matter	[kg·m^{-3}]	eq. (18)
$PEC_{local, sed}$	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 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.

2.6.6. 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.

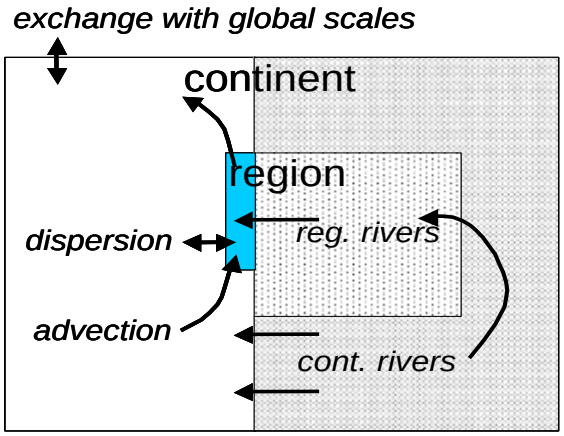
Point source releases may have a major impact on the environmental concentration on a local scale (PEC_{local}) and contribute to the environmental concentrations on a larger scale ($PEC_{regional}$). Like with the freshwater environment for the marine situation it is necessary to evaluate the impact of substances that are released from point and diffuse sources over a wider area. The $PEC_{regional}$ is supposed to take into account the further distribution and fate of a chemical upon release. The resulting $PEC_{regional}$ 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 points and diffuse sources of substances on the marine environment a river plume in coastal seawater 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. 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 zoneand the continental seawater. 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 $PEC_{regional}$ for the freshwater environment (Section 2.3.8.7 of this Guidance.)[12].

The calculation of $PEC_{regional}$ according to this scenario provides the results for the risk assessment that is necessary for the evaluation for active substances. 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

[12] 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 seawater 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 waters (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.

K_{ow}. 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.

3. Effects and Hazard Assessment

3.1. Introduction

The environmental effect and hazard assessment is a required step in the risk assessment. It is based on information to be submitted as detailed in Part A of Volume IV on:

- physical and chemical data;
- fate and behaviour in the environment (including degradation and mobility);
- effects on aquatic organisms (including sediment-dwellers);
- effects on terrestrial organisms (including mammals and birds).

Using the data above, a PNEC has to be derived for all relevant environmental compartments:

- fresh water aquatic ecosystem (including the sediment);
- marine aquatic ecosystem (including the sediment);
- terrestrial ecosystem (including groundwater);
- microbial activity in a sewage treatment plant;
- primary/secondary poisoning (predators).

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 $L(E)C_{50}$ or long term NOEC value by an appropriate assessment factor.

The following Table provides and overview of toxicity test endpoints that can be used for deriving PNEC values.

Table 18: Overview of toxicity test endpoints

Short-term studies:
If a test report does not indicate the $L(E)C_{50}$ values but the raw data are presented, the $L(E)C_{50}$ should be calculated, for example by Probit analysis. If only one toxicity value lies between the $L(E)C_0$ and the $L(E)C_{100}$, the $L(E)C_{50}$ cannot be calculated by Probit analysis. Instead, the $L(E)C_{50}$ may be estimated by, e.g., linear regression. If results are presented as $>L(E)C_{10}$ and $<L(E)C_{50}$, they can be rated as $L(E)C_{50}$ while results clearly above a $L(E)C_{50}$ 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. The NOEC is determined directly from the concentration-effect curve by consideration of the deviation of the control (e.g. 10%) or derived on the basis of ANOVA (analysis of variance) and a subordinate test (e.g. Dunett's). An EC_{10} for a long-term test which is obtained by extrapolation using appropriate statistics (e.g. Probit analysis) can be considered as a NOEC. The choice between the NOEC or EC_x point estimates is subject of continuing debate. OECD (1998) favours the use of an EC_x. Extensive information on the implications of either choice for test set-up and statistical evaluation is given by OECD (2006). 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/EC_{10}. In case only a LOEC is given in the report, it can be used to derive a NOEC/EC_{10} with the following procedures:

- LOEC > 10 and < 20% effect: NOEC can be calculated as LOEC/2.
- LOEC ≥ 20% effect and a distinct effect relationship: the EC_{10} 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 may be 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 √2 to derive a NOEC.

It should be noted that in the case of algae studies, which are actually multigeneration studies, it is generally accepted that a 72-hour (results from shorter or longer test can be used provided that all validity criteria are met) EC_{50} value may be considered as equivalent to a short-term result and that a 72-hour (or longer) NOEC/EC_{10} value can be considered as a long-term result.

The assessment factor is an expression of the degree of uncertainty when extrapolating from test data 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. Results from field tests or mesocosm studies can also be used to derive a PNEC on a case by case basis (Appendix 8).

In specific cases where it is not possible to establish a PNEC, a qualitative estimate has to be made.

If, during the transformation of the substance, relevant metabolites/transformation products are formed (see Infobox 1), an effect assessment for the concerned compartments will have to be carried out.

The effects and hazard assessment comprises the following steps:

- hazard identification: The aim of the hazard identification is to identify the effects of concern in the different species of each environmental compartment. For active substances and substances of concern, the aim is also to re-assess the classification and labelling of the substance. For new active substance the classification and labelling is still to be established;
- dose (concentration) - response (effect) assessment: The aim is to calculate the values for each endpoint tested. At this step the predicted no effect concentration (PNEC), must, where possible, be determined.
- As a new requirement under the BPR, there is need to assess if an active substance fulfills the exclusion criteria according to Article 5(1) of the BPR. PBT/vPvB criteria and endocrine disrupting properties need to be evaluated for the assessment of the exclusion criteria (see Section 3.11 of this Guidance).

For the different 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 must address the quality and relevance of data (see Section 3.2 of this Guidance). The evaluation of data is of particular importance where non standard organisms and/or non-standardised methods are used. It is suitable to start the effects assessment process with the evaluation of the available ecotoxicological data.

The environmental compartments considered for the inland environment are the aquatic and terrestrial ecosystem, predators, microbial activity in a STP, and the atmosphere. This means that for each of these compartments a PNEC has to be derived.

In the case of the aquatic environment, a detailed description on deriving a $PNEC_{water}$ is described in Section 3.3 of this Guidance. For an intermittent release of substances, aquatic organisms may be exposed for only a short period. In these cases, short-term $L(E)C_{50}$ values are considered sufficient to derive a $PNEC_{water\text{-}intermittent}$. This is described in Section 3.3.2.

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

For the sediment compartment, the equilibrium partitioning method is proposed as a screening method for derivation of a $PNEC_{sediment}$. If sediment test results are available, the $PNEC_{sediment}$ is derived from these data by applying assessment factors (see Section 3.5 of this Guidance).

When assessing the soil compartment, if test data are lacking, also the equilibrium partitioning method can be used to derive a $PNEC_{soil}$. If soil test results are available, the $PNEC_{soil}$ is derived from these data by applying assessment factors (see Section 3.6 of this Guidance).

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 of this Guidance.

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 an active substance 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 ($PEC_{oral,\ fish}$ and $PEC_{oral\ worm}$) is compared to a PNEC for fish- or worm-eating mammals or birds. This approach is described in Section 3.8 of this Guidance.

In addition to the 'secondary poisoning', in some cases primary poisoning (e.g. for rodenticides or PT insecticides), may take place and needs to be assessed. Please refer to the PT-specific ESDs and -guidance for further information and to Appendix 6 of this document.

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 active substance. 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

As mentioned previously, during the effect and hazard assessment, it is required to evaluate data with regard to their adequacy and completeness. Details on the evaluation of completeness and adequacy of ecotoxicity data is provided in Part A of Volume IV.

Infobox 5: Derivation of PNEC values

Derivation of PNEC values from studies with no effects at the highest test concentration

When there are no effects at the highest test concentration, a "≥" symbol should be used for expressing the NOEC-value. If at the highest test concentration <50% effect is observed, a ">" sign should be used to express the LC/EC_{50}. If a PNEC value is to be derived from such a value, the assessment factor (AF) is applied to that value and the PNEC presented with the > sign. Example: LC_{50} >100 mg/L, and an assessment factor of 1000 gives a PNEC >0.1 mg/L. Combining this with a PEC of (e.g.) 1 mg/L, the risk quotient is represented as RQ <10. Note that in some cases it may be possible to derive an LC/EC_{10} from the data, which may be used for PNEC derivation instead of a NOEC.

Use of efficacy data on target species to derive a PNEC value

Information from efficacy tests can be used to define the potentially most sensitive taxonomic group, which may trigger a need for additional information. However, ecotoxicological data can only complemented with results from efficacy tests if these fulfil the design criteria for ecotoxicity tests like those described in OECD guidelines.

3.2.2. Quantitative Structure-Activity Relationships (QSAR)

Means of obtaining reliable QSAR estimates for fish, Daphnia and algal toxicity are available for many chemicals. 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. It is also a valuable tool when assessing metabolites and degradation products where no laboratory tests are available. R.6: QSARs and grouping of chemicals, (ECHA, 2008) gives full details on the use of QSAR estimates within the testing strategy for:

- predicting the toxicity of chemicals; and
- predicting long-term fish toxicity.

3.3. Effects assessment for the freshwater 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 groups, and;

- protecting ecosystem structure protects community function.

These two assumptions have important consequences. By establishing which species are the most sensitive to the toxic effects of a chemical in the laboratory, extrapolation can subsequently be based on the data from those species. Furthermore, the functioning of any ecosystem in which those species exist 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 groups should protect structure, and hence function.

For most substances, the pool of data from which to predict ecosystem effects is limited as, in general, only single species laboratory 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 $PNEC_{water}$ 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 core data set. Calculation of a PNEC using assessment factors is described in Section 3.3.1.1 of this Guidance.

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 of this Guidance.). 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 in rare cases 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 19.

When only short-term toxicity data are available, an assessment factor of 1000 will be applied on the lowest $L(E)C_{50}$ of the relevant available toxicity data, irrespective of whether or not the species tested is a standard test organism (see notes on Table 19). A lower assessment factor will be applied on the lowest $NOEC/EC_{10}$ derived in long-term tests with a relevant test organism.

For some compounds, a large number of validated short-term $L(E)C_{50}$ values may be available. Therefore, it is proposed to calculate the geometric mean if more than one $L(E)C_{50}$ 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 core data set is in principle a multigeneration test. However, for the purposes of applying the appropriate assessment factors, the EC_{50} is treated as a short-term toxicity value. The NOEC/EC_{10} from this test may be used as an additional NOEC/EC_{10} when other long-term data are available. In general, an algal NOEC/EC_{10} should not be used unsupported by long-term NOEC/EC_{10} 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/EC_{10} from this test should be supported by the result of a test on a second species of algae. Blue-green algae should be counted among the primary producers due to their autotrophic nutrition.

The assessment factors presented in Table 19 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 core data set species;
- the availability of test data from a variety of species covering the taxonomic groups of the core data 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 19.

Table 19: Assessment factors to derive a $PNEC_{water}$

Available data	Assessment factor
At least one short-term L(E)C_{50} from each of three trophic levels (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[g])	50 [c)]
Long-term NOECs from at least three species (normally fish, Daphnia and algae[g]) 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 on Table 19:

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 of this Guidance).
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)C_{50} in the short-term tests. It is further assumed that no NOEC/EC_{10} for algae is available.
If the only available long-term NOEC/EC_{10} is from a species (standard or non-standard organism) which does not have the lowest L(E)C_{50} 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/EC_{10} available.
An assessment factor of 100 applies also to the lowest of two long-term NOECs/EC_{10} covering two trophic levels when such NOECs/EC_{10} have not been generated from that showing the lowest L(E)C_{50} of the short-term tests. This should, however, not apply in cases where the acutely most sensitive species has an L(E)C_{50} 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)C_{50} of the short-term tests.

c) An assessment factor of 50 applies to the lowest of two NOECs/EC_{10} covering two trophic levels when such NOECs/EC_{10} have been generated covering that level showing the lowest L(E)C_{50} in the short-term tests. It also applies to the lowest of three NOECs/EC_{10} covering three trophic levels when such NOECs/EC_{10} have not been generated from that trophic level showing the lowest L(E)C_{50} in the short-term tests. This should however not apply in cases where the acutely most sensitive species has an L(E)C_{50} value lower than the lowest NOEC/EC_{10} value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C_{50} of the short-term tests.

d) An assessment factor of 10 will normally only be applied when long-term toxicity NOECs/EC_{10} 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 $PNEC_{water}$ should be calculated from the lowest available NOEC/EC_{10}. 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/EC_{10} 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/EC_{10} 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 of this Guidance.

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.(Further information on the use of mesocosms for biocides can be found in Appendix 8)

*derived from a fish early life stage (FELS) test or fish full life cycle (FFLCT) test. Under certain conditions also a fish juvenile growth test (for substances with a log K_{ow} < 5) or a fish short-term toxcitiy test on embryo and sac fry stages (for substances wit a log K_{ow} < 4) can cover long-term toxicity to fish.

For compounds with a high log K_{ow} no short-term toxicity may be found. In these cases it may indeed be difficult to maintain the exposure concentration in the test system due to the partitioning of test substances in the test system. This may be the case also in long-term tests in which the steady state may not be reached. In fish tests for non-polar narcotics, this can be substantiated by the use of long-term QSARs (see Section 3.2.1.2 of this Guidance and *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*. 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 K_{ow} > 3 (or BCF > 100) and if the PEC_{local} is > 1/100th of the water solubility. 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 core data 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 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 statistical extrapolation for regulatory purposes 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.

<u>Input data</u>

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).

<u>Which taxonomic groups</u>

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 SSD 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.

According to Brock et al. (2011), measurement parameters, from which endpoints are calculated, should preferably be sensitive/responsive in the range of tested concentrations such that SSDs avoid the use of greater- or lower-than values. In general, it is not recommended to include unbound values (greater-than or lower-than values) in the SSD. There are situations, however, where ignoring those data would lead to a loss of valuable information. When a lower-than value is lower than the lowest toxicity endpoint, this means that the other data do not cover the whole range of sensitivities. Leaving out this information might lead to a lower limit, median and upper limit hazardous concentration to 5% of the species (HC5) that is underprotective.

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 instance, particular attention should be given to the conditions which may justify the differences in the obtained results: e.g concentrations tested in the various studies, different life stages of the species tested in different tests, different exposure durations, etc., which may justify the differences in the results obtained. 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.

Infobox 6: Treatment of data if there is more than one test result available for the same species

It is stated above that if the same species is tested on the same endpoint with the same test duration, the geometric mean value should be used for the derivation of the PNEC. However, "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". Differences in the test design (static, flow-through, analytical monitoring) may influence the result of a study and thus may limit the possibility to derive a geometric mean value.

Fit to a distribution

Logistic and log normal distributions are most often used, because they require less data than distribution-free methods and are relatively easy to fit with standard statistical software (Aldenberg and Jaworska, 2000; Aldenberg et al., 2002; Van Vlaardingen et al., 2004). However, while it is typically assumed that SSDs follow a lognormal distribution, significant deviation from normality (whether log transformed or not) should be a trigger for trying other distributions, (e.g. Burr type III, Weibull) that may provide a better goodness of fit. Techniques such as bootstrapping have been avoided, since they do not meet the assumption of normality, but if sample size is sufficiently large then (non-)parametric bootstrapping methods may provide point estimates and confidence intervals that are fit for purpose. Please note that there are many ways of calculating 5th percentiles, but the methods presented by Aldenberg and Jaworska (2000), Aldenberg et al. (2002) and Van Vlaardingen et al. (2004) provide 5th percentiles taking into account the sample size and also allowing the calculation of the uncertainty around the calculated 5th percentile.

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:

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

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 (see Appendix 8), 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 (see Appendix 8); in any case a PNEC should also be derived 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 of this Guidance 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 $PNEC_{water\text{-}intermittent}$, therefore, generally only short-term studies need to be considered. It is therefore proposed that, to derive a $PNEC_{water\text{-}\ intermittent}$ for such situations, an assessment factor of 100 be normally applied to the lowest $L(E)C_{50}$ 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 $L(E)C_{50}$ 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 $PNEC_{stp}$. The $PNEC_{stp}$ 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 EC_{50} values determined for test substances using a variety of tests (EU Annex V C.11, OECD 209, 1984f, EU Annex V C.4F, Closed Bottle Test, Growth Inhibition) were found to be inhibitory in ready biodegradability tests (EU Annex V C.4C,F,E,B; OECD 301B,C,D,E, 1992f). No-effect or EC_0 values were 1.5 to 10 times lower than the corresponding EC_{50} values. The authors recommend as a provisional rule that biodegradation testing should therefore be conducted at one-tenth of the EC_{50} 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 $PNEC_{stp}$. 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 $PNEC_{stp}$. 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 $PNEC_{stp}$. 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 $PNEC_{stp}$ 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 $PNEC_{stp}$ 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 of this Guidance). 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 $PNEC_{stp}$ should be obtained as a first step in the effects assessment for microorganisms in both domestic and industrial sewage treatment plants.

The $PNEC_{stp}$ 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 $PNEC_{stp}$ 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, the Shk1 Assay (activated sludge bacterial luminescence inhibition assay). An EC_{50} from this test is divided by an assessment factor of 10;
- An assessment factor (AF) of 10 is to be applied to the NOEC of a sludge respiration test, reflecting the lower sensitivity of this endpoint as compared to nitrification, as well as the short duration of the test. The corresponding AF is 100 when based on the EC_{50};
- the lowest value is selected as the $PNEC_{stp}$.
- If no standard microbial inhibition test data are available, the $PNEC_{stp}$ can also be derived from available ready biodegradation tests. An assessment factor of 10 is applied to the test concentration at which no toxicity to the inoculum was observed. This approach can also be used for inherent biodegradability tests.
- From an activated sludge simulation study, a $PNEC_{stp}$ can be derived based on the PEC_{stp} or $PEC_{influent}$. The AF of 1 can be used in case there is no impact on nitrification and BOC/COD removal performance (NB: if sludge from an industrial WWTP was used for the test, the $PNEC_{stp}$ can not be used for the extrapolation to a domestic STP).
- No AF is needed to derive a $PNEC_{stp}$ based on good quality field data as this has to be assessed by expert judgement.

There may be cases in which the lowest $PNEC_{stp}$ 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 $PNEC_{stp}$. Usually the effect value of the most sensitive test system should be used as a basis for the calculation of $PNEC_{stp}$ employing the appropriate AF.

Table 20 provides a complete listing of the test systems mentioned above, effect concentrations that are determined using them and the corresponding assessment factors.

Table 20: Test systems for derivation of $PNEC_{stp}$

Test	Available value	Assessment factor
Respiration inhibition tests	NOEC or EC_{10}	10
EU Annex V C.11; OECD 209 (1984f) ISO 8192 (1986)	EC_{50}	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	NOEC or EC_{10}	1
ISO-9509 (1989)	EC_{50}	10
Ciliate growth inhibition tests	NOEC or EC_{10}	1
(preferably with Tetrahymena, cf. OECD, 1998a) [1)]	EC_{50}	10
Activated sludge growth inhibition tests	NOEC or EC_{10}	10
ISO-15522	EC_{50}	100
Pilot scale activated sludge simulation tests	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: 10 down to 1 (for a well executed and documented test)*
OECD 303A (2001b) ISO-11733		
Growth inhibition test with Pseudomonas putida	NOEC or EC_{10}	1
NF EN ISO 10712 (1995)	EC_{50}	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 seawater species	

*A higher AF (i.e. 10) can be applied in case of badly executed tests

Notes on Table 20:

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

If on the basis of the $PNEC_{stp}$ 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 $PNEC_{stp}$:

- 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 $PNEC_{stp}$ for this specific site can be derived from a nitrification inhibition test using sludge from this site's STP. The revised $PNEC_{stp}$ 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 $PNEC_{stp}$ 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 $PNEC_{stp}$ for a specific industrial STP is derived from these tests using the assessment factors described above for respiration inhibition tests. A $PNEC_{stp}$ 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 $PNEC_{stp}$ 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 $PNEC_{stp}$ is not available.

Infobox 7: Derivation of $PNEC_{stp}$ for active substances where the EC_{50} values exceed the water solubility

If significant inhibition is observed in the test, when concentrations higher than the water solubility are used, the test result (EC_{50}) is used to derive a $PNEC_{stp}$.
If no inhibition is observed at the highest test concentration, the NOEC is set equal to the water solubility which is subsequently used to derive the $PNEC_{stp}$. If then a risk is indicated the assessment should be refined.

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.

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

General recommendations on the risk assessment for sediment compartment are available at the Proceedings of the ECHA Topical Scientific Workshop on Risk Assessment for the Sediment Compartment [http://echa.europa.eu/view-article/-/journal_content/title/topical-scientific-workshop-on-risk-assessment-for-the-sediment-compartme-1].

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, seawater sediment effects assessment is necessary for substances that are known to be persistent in seawaters, 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 of this Guidance;
- 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 of this Guidance.

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 of this Guidance). 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 21 presents an overview of different data configurations and explains how to use them for the risk characterisation for sediment.

Table 21: Requirements for performing a risk characterisation for sediment

Available measured data: PECsed	Available measured data: PNECsed	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)

Infobox 8: Normalisation to default organic matter for freshly deposited sediment

When test are available on the sediment compartment, the endpoint should be reported in dry weight (as recommended by the OECD 218) and consequently the $PNEC_{sed}$ will be expressed in dry weight. This means no correction procedure would be needed on the effects endpoint. Then the PEC should be converted to dry weight by:

a) Replacing the RHOss (wet) of 1150 kg wwt/m³ with RHOss (dry) 250 kg dwt/m³ in the formula for the PEC_{sed}.

b) Keeping RHOss (wet) to calculate a PEC wet weight and then convert it to dry weight using the default conversion factor of 4.6 kgwwt/kgdwt.

3.5.3. Calculation of PNEC using equilibrium partitioning

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

It has to be considered that the EPM may result both in an overestimation or underestimation of the toxicity to benthic organisms (Di Toro et al. 2005). Therefore this method can only be used as rough screening to decide whether sediment toxicity tests with benthic organisms are required.

In the EPM, 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 of this Guidance).

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

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

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 K_{ow} greater than 3. For these compounds the total uptake may be underestimated;
- for compounds with a log K_{ow} greater than 5 or with a corresponding adsorption or binding behaviour not triggered by the lipophilicity (e.g. log K_{ow}) of the substance but by other mechanisms (e.g. ionisable substances, surface active substances, substances forming covalent bound to sediment, components like e.g. aromatic amines) a modified equilibrium method is used.

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

Sediment assessment has been traditionally limited to sediment invertebrates, but other taxonomic groups and sediment functions may be also relevant. Getting a proper coverage is particularly relevant for biocides, which have specific modes of action frequently leading to high sensitivity for certain taxonomic groups. Current OECD Test Guidelines are limited to sediment dwelling invertebrates, although other taxonomic groups are covered by other standard guidelines. If the information available confirms that invertebrates are expected to be among the most sensitive group, an assessment focusing on this group with the AFs indicated in Table 22 is sufficient.The selection of species/taxa and of feeding behaviour and triads should also consider the biocidal mode of action. In general, tests should be

conducted with spiked sediment and following the recommendations for ensuring that dietary exposure is properly covered during the test.

The $PNEC_{sediment}$ is derived from the lowest available NOEC/EC_{10} obtained in long-term tests by application of the following assessment factors (Table 22):

Table 22: Assessment factors for derivation of $PNEC_{sed}$

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

If other taxonomic groups or environmental functions are expected to be of higher sensitivity, a case-by-case assessment is needed, and a comparison with a PNEC based on equilibrium partitioning may be considered. Mesocosms studies may offer adequate coverage if the relevant endpoints are measured. Further guidance on the use of mesocosm studies for biocides can be found in Appendix 8).

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, manure application, direct application of chemicals by means of spraying, leaching 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 groundwater 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 Volume IV, Part A (Information requirements) applies.

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 of this Guidance) and for bioaccumulation and secondary poisoning of birds and mammals (Section 3.8 of this Guidance).

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 and toxicity tests with terrestrial organisms may be required for biocides depending on product-type and expected use.

When no toxicity data are available for soil organisms or if experimental data are missing for the potentially most sensitive species group, the equilibrium partitioning method can be applied to aquatic data to identify a PNEC for soil organisms. However, this method cannot replace required core toxicity data for soil organisms and should only be considered as a "screening approach" 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).

Tests on microorganisms using the two test concentrations with a control can be used for the environmental risk assessment of biocides in special circumstances. First, a statistical evaluation (student t-test) of difference of the test concentrations to the control is conducted. If no statistical difference is found in both tested concentrations the highest concentration can be used as NOEC. If a statistical difference is analysed and the effect is >15 % no NOEC can be derived. The test cannot be used for assessment under the BPD and, if the test is critical for the assessment, a new test using 5 concentrations needs to be requested. If in at least one concentration no statistical difference from the control is found and the effect value is ≤ 15 % the concentration is the NOEC.

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, may be influenced by the soil properties. This means that results from different test soils may not 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 of this Guidance).

Infobox 9: Correction of ecotoxicological test results with soil organisms to the standard soil with an organic matter content of 3.4 %

All effect concentrations from terrestrial plants and terrestrial microorganisms should normally be converted to the standard organic matter (see Table 5) before choosing one effect value for derivation of PNEC. For non-ionic organic compounds the normalization is considered appropriate assumed that the binding behaviour of the substance in question is predominantly driven by its log K_{ow}, and that organisms (except earthworm) are exposed predominantly via pore water.

For non-ionic organic compounds it is assumed that bioavailability is determined by the organic matter content only. NOECs and L(E)C_{50}s are corrected according to the formula:

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

Explanation of symbols

NOEC or L(E)$C_{50,\ exp}$	NOEC or L(E)C_{50} in experiment	[mg·kg^{-1}]	
$F_{om,\ soil(standard)}$	fraction organic matter in standard soil	[kg·kg^{-1}]	Table 5
$F_{om,\ soil(exp)}$	fraction organic matter in experimental soil	[kg·kg^{-1}]	
NOEC or L(E)$C_{50,\ standard}$	NOEC or L(E)C_{50} in standard soil	[mg·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 log K_{ow}, and that organisms are exposed predominantly via pore water.

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

- terrestrial toxicity data are a product-type specific information requirement for some of the PT. However, when no toxicity data are available for soil organisms, or if experimental data are missing for the potentially most sensitive species group, 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 of this Guidance (see also Section 3.5.2 sediment of this Guidance);
- 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 of this Guidance; provided that the potentially most sensitive taxon is not included in the test species; the previous bullet point still applies.
- When only test results for a single soil dwelling species are available the risk assessment is performed both on the basis of this result using assessment factors and on the basis of the EPM. From both $PEC_{soil}/PNEC_{soil}$ ratios the highest one is chosen for the risk characterisation.

3.6.2.1. Calculation of PNEC using equilibrium partitioning

The EPM is based on the assumption that soil toxicity expressed in terms of the freely-dissolved substance concentration in the pore water is the same as aquatic toxicity. The pore water concentration is correlated with the bioavailable fraction. Although Di Toro *et al.* (1991) based their analysis on sediment partitioning the rationale can also be applied to soils. However 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.

The equilibrium partitioning method may not be suitable for highly lipophilic substances or substances with a specific mode of action nor for organisms that are exposed primarily through food (Van Gestel, 1992). However, for Collembola and Oribatid mites, there are indications that direct exposure to soil may be of much greater importance for uptake than is exposure via the food (Løkke and van Gestel, 1998).

It should be recognised that substitution of terrestrial toxicity data by aquatic toxicity data should be used with caution. 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 and may only be appropriate for organisms with a water-permeable epidermis. Furthermore, studies have shown that the equilibrium partitioning method can give significant over- or underestimations, due to inaccurate partitioning coefficients or differences in species sensitivities. Therefore, further research is required into the general applicability of the EPM for other organisms.

Therefore, if the $PEC_{soil}/PNEC_{soil}$ ratio calculated using the EPM is greater than 1, tests with soil organisms should be considered as an essential requirement for a refined effects assessment. Alternatively, the PEC could also be refined. 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)
$K_{soil\text{-}water}$	partition coefficient soil water	$[m^3 \cdot m^{-3}]$	eq. (24)
$PNEC_{soil}$	Predicted No Effect Concentration in soil	$[mg \cdot kg^{-1}]$	

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 K_{ow} > 5 (or for compounds with a corresponding adsorption or binding behaviour, e.g. ionisable substances).

EPM probably overestimates the actual uptake from soil by soil invertebrates (Jager, 2004). However, this relation is complicated and probably depends on the ability to properly calculate the dissolved concentration in the soil. Therefore it is considered that the possible overestimation of exposure is acceptable when using the equilibrium partitioning method for chemicals with a log K_{ow} between 3 and 6;

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).

3.6.2.2. Calculation of PNEC using assessment factors

The same assessment factors used for the aquatic compartment (see Table 19) are applied to the terrestrial compartment (see Table 23). 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. The choice of taxonomic groups for which toxicity data are necessary (conform to the core data set of algae, Daphnia and fish for the aquatic environment), is a point of discussion. A dataset comprising of toxicity data for primary producers, consumers and decomposers is preferred.

The assessment factors for the PNEC determinationare reported in Table 23.

Table 23: Assessment factors for derivation of $PNEC_{soil}$

Information available	Assessment factor
L(E)C_{50} 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
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, or a decomposer are available (e.g. plants, earthworms, or microorganisms), 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 23 should be applied.

Infobox 10: Clarifications on the assessment factor to derive PNECsoil

Test with plants described in OECD TG 208 or OECD TG 227: Can this test be considered as a short or long term test and how does this influence the assessment factor to derive the $PNEC_{soil}$?

Different interpretations exist on whether this test can be considered as a short or a long term study. The study is in principle a short-term study; however, it was decided that it also can be considered a long-term study under certain circumstances, provided that in addition to the EC_{50} also a NOEC/EC_{10} was derived from this test. Depending on the sensitivity of plants compared to other taxonomic groups when comparing L(E)C_{50} values, different assessment factors to derive the PNECsoil must be chosen (for details see "Choice of AF for PNECsoil derivation", below).

Possibility to lower the assessment factor for the derivation of the $PNEC_{soil}$ from 1000 to 100 when the most sensitive species is unknown (e.g. data for micro-organisms and acute data for earthworms are available, but no data for plants)

Application of an assessment factor of 100 instead of 1000 is only possible when effect data for three different species (i.e. micro-organisms, earthworms and plants) are available and therefore the potentially most sensitive species can be established (for details see "Choice of AF for PNECsoil derivation", below).

In specific situations, and on a case by case basis, when the necessary data to establish the most sensitive species is available from a very similar compound as the active substance under consideration, and can be extrapolated, than these data can be used to lower the assessment factor to 100.

Choice of AF for PNECsoil derivation

If test results are available for:

- Microorganisms (28 days EC_{50} and NOEC/EC_{10})
- Plants (EC_{50} and NOEC/EC_{10} according to e.g OECD 208)
- Earthworms (14 days LC_{50} and 56 days NOEC/EC_{10}),

three different situations can be distinguished with respect to PNEC derivation and the choice of the AF:

1. Acutely, plants are not the potentially most sensitive species (EC_{50} ≥ 10 times higher than $L(E)C_{50}$ for microorgansims and/or earthworms): An AF of 10 should be applied to the lowest $NOEC/EC_{10}$ for either microorganisms, plants or earthworms.

2. Acutely, plants are the potentially most sensitive species but the plant EC_{50} is ≥ 10 times higher than the $NOEC/EC_{10}$ from either the microorganism or the long-term earthworm study: An AF of 50 should be applied to the lowest $NOEC/EC_{10}$ for earthworm or microorganism.

3. Acutely, plants are the potentially most sensitive species and the plant EC_{50} is significantly* lower than the $NOECs/EC_{10}$ from the microorganism and the long-term earthworm study: An AF of 100 should be applied to the lowest $L(E)C_{50}$ (in analogy to the PNEC derivation for the aquatic compartment).

These assessment factors can be reduced if further testing on chronic toxicity to plants, e.g. according to ISO standard 22030:2005 on determining the inhibition of the growth and reproductive capabilities of higher plants, becomes available.

* Endpoints are considered not to be significantly different when the sensitivity difference is within a factor of less than 10 (according to TGD).

Infobox 11: Presentation of recalculations of effect results (e.g. NOEC values) expressed as a.s./ha

Any recalculations necessary for the effects assessment should be explained and performed in the effects assessment section of the Assessment Report. Consequently, conversion of a test result expressed as active substance/ha to for example mg/kg must be presented in Part A/B of Section 2 of the Assessment Report. If information on test conditions (i.e. soil density, structure, type of soil, etc) is available, then this should be used for the recalculation to mg/kg. If no information can be derived from the test, a default soil depth of 10 cm and soil density of 1500 kg/m³ dry soil should be used. The original expression of the study results will be maintained in IUCLID.

Infobox 12: How to deal with studies with terrestrial microorganisms that were performed using the PPP design (2 test concentrations with a control)

Tests using the PSM design (two test concentrations with a control) can be used for the environmental risk assessment of biocides in special circumstances. First, a statistical evaluation (student t-test) of difference of the test concentrations to the control is conducted. If no statistical difference is found in both tested concentrations the highest concentration can be used as NOEC. If a statistical difference is analysed and the effect is >15% no NOEC can be derived. The test cannot be used for assessment under the BPD and, if the test is critical fort he assessment, a new test using a 5 concentrations needs to be requested. If in at least one concentration no statistical difference from the control is found and the effect value is </= 15% the concentration is the NOEC. The NOEC micro-organisms can be used to derive the PNEC soil by using an AF of 100 even if no other NOEC's for soil organisms are available.

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. SSDs can obly be performed when at least 10 NOECs (and preferably 15 NOECs) are avaulabe from at least 8 taxonomic groups. 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 LC_{50} 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 substances 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 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 is expected 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. Please see also Annex I and II of Regulation (EC) No 1005/2009 of the European Parliament and of the Council of 16 September 2009 on substances that deplete the ozone layer. 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, CH_4) 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 Section 4.5.1 of this Guidance. 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 BCF at any time during the uptake phase of this accumulation test is the concentration of test substance in/on the fish or specified tissues thereof (Cf as mg/kg) divided by the concentration of the chemical in the surrounding medium (Cw as mg/L). BCF is expressed in l/kg-1. Please note that corrections for growth and/or a standard lipid content are not accounted for. The steady-state bioconcentration factor (BCF_{SS}) does not change significantly over a prolonged period of time, the concentration of the test substance in the surrounding medium being constant during this period. The kinetic bioconcentration factor (BCF_K) is the ratio of the uptake rate constant, k_1, to the depuration rate constant, k_2 (i.e. k_1/k_2 – see corresponding definitions in Annex 1 of the OECD TG 305). In principle the value should be comparable to the BCF_{SS} (see definition above), but deviations may occur if steady-state was uncertain or if corrections for growth have been applied to the kinetic BCF. The lipid normalised kinetic bioconcentration factor (BCF_{KL}) is normalised to a fish with a 5 % lipid content. The lipid normalised, growth corrected kinetic bioconcentration factor (BCF_{KgL}) is normalised to a fish with a 5 % lipid content and corrected for growth during the study period as described in Annex 5 of the OECD TG 305. The dynamic bioconcentration factor can be calculated as follows:

$$BCF_{fish} = \frac{C_{fish}}{C_{water}} \quad or \quad \frac{k_1}{k_2} \tag{73}$$

Explanation of symbols

C_{fish}	concentration in fish	$[mg \cdot kg_{ww}^{-1}]$
C_{water}	concentration in water	$[mg \cdot l^{-1}]$
k_1	uptake rate constant from water	$[l \cdot kg_{ww}^{-1} \cdot d^{-1}]$
k_2	elimination rate constant	$[d^{-1}]$
BCF_{fish}	bioconcentration factor	$[l \cdot kg_{ww}^{-1}]$

At the core data 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 (see Section 3.8.3 of this Guidance). For the terrestrial ecosystem a similar strategy is used which is described in Section 3.8.3.7 of this Guidance.

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. But also results from bioaccumulation studies in aquatic species can be used. Determination of the BCF alone, however, only gives a partial picture of the potential of bioaccumulation,results from a bioaccumulation study in terrestrial species, data from scientific analysis of human body fluids or tissues, such as blood, milk, or fat; detection of elevated levels in biota, in particular in endangered species or in vulnerable populations, compared to levels in their surrounding environment; results from a chronic toxicity study on animals; assessment of the toxicokinetic behaviour of the substance; information on the ability of the substance to biomagnify in the food chain, where possible expressed by biomagnification factors (BMF) or trophic magnification factors (TMF) can be used to assess the bioaccumulation potential in addition to experimental measurements of the BCF or BMF. 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 K_{ow} 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 K_{ow} value. A survey of these factors is given below.

n-Octanol/water partition coefficient

At the core data set level, the potential for bioaccumulation can be estimated from the value of the *n*-octanol/water partition coefficient, log K_{ow}, this parameter should be determined experimentally. If the test cannot be performed for the physico-chemical properties of the substance, then, a calculated value for log P as well as details of the calculation method must be provided. (See REACH endpoint specific guidance R7a (7.1.8) for more detail).

It is accepted that values of log K_{ow} 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 K_{ow} 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 K_{ow} 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 K_p > 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 readily biodegradable substances concentrations will be low in aquatic organisms.

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, but molecular weight alone is insufficient to demonstrate limited bioaccumulation potential. These substances are unlikely to bioconcentrate significantly (regardless of the log K_{ow}-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 a substance:

- has a log $K_{ow} \geq 3$; or;
- has a BCF ≥ 100 L/kg_{ww}; or;
- has a BAF ≥ 100 L/kg_{ww}; or;
- has a BMF >1; 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 log K_{ow}. The test guidelines also contain information on the suitability of the various log K_{ow} determination methods depending on the type of substance concerned. Further information on octanol-waterpartition coefficient and in bioaccumulation can also be found in the *Guidance on information requirements and chemical safety assessment Chapter R.7a*, *Endpoint specific guidance,* section 7.1.8 and R.7c, section R.7.10 and R.11.

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 $K_{ow} < 4.5$ 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 $K_{ow} \geq 4.5$, 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 $\rightarrow$ aquatic organisms $\rightarrow$ fish $\rightarrow$ 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 and monitoring data 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 16.

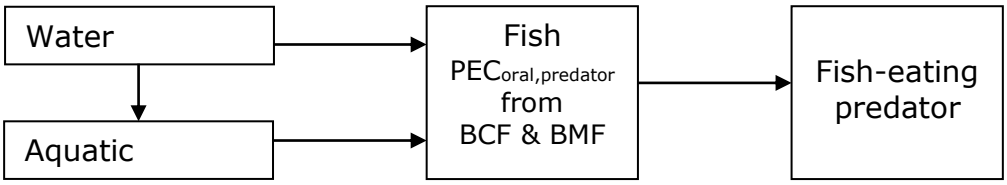


Figure 16: Assessment of secondary poisoning

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 ($PEC_{oral,\ predator}$) 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, $PEC_{oral,\ predator}$ is calculated from the bioconcentration factor (BCF) and a biomagnification factor (BMF). Note that $PEC_{oral,\ predator}$ 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 K_{ow}

If measured BCF values are not available, the BCF for fish can be predicted from the relationship between K_{ow} and BCF. Various methods are available to calculate K_{ow}, such as:

- Quantitative structure-activity relationships (QSARs);
- Expert systems; and
- Grouping approaches (including read-across, structure-activity relationships (SARs) and chemical categories).

Often a large variation is found in the K_{ow} values of a chemical by using different methods. Therefore the K_{ow}-value must have been evaluated by an expert. For substances with a log K_{ow} 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

K_{ow}	octanol-water partition coefficient	[-]
BCF_{fish}	bioconcentration factor for fish on wet weight basis	[l·$kg_{wet\ fish}$]

For substances with a log K_{ow} 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

K_{ow}	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 molecular weight less than 700.

3.8.3.3. Experimentally derived BCF

Traditionally, bioconcentration potential has been assessed using laboratory experiments that expose fish to the substance dissolved in water. 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, 2012). Dietary bioaccumulation tests might be better considered for adsorptive and poorly water-soluble substances (when it is technically not feasible to test), than the OECD 305 guideline, because a higher and more constant exposure to the substance can be administered via the diet than via water. A further advantage is that multiple substances, including mixtures, can be investigated in a single test.

The following parameters may be of importance when considering the results of testing:

- BCF (bioconcentration factor);
- CT_{50} (clearance time, elimination or depuration expressed as half-life);
- metabolism/ transformation;
- organ-specific accumulation (reversible/ irreversible);

- incomplete elimination (bound residues);
- substance bioavailability.

Past work has shown that tests with substances with a high log K_{ow} 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) or the REACH *Guidance on information requirements and chemical safety assessment, R.7.10.3.1. and R.11* 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 ($PEC_{oral,\ predator}$) is calculated from the PEC for surface water, the measured or estimated BCF for fish and the biomagnification factor (BMF):

$$PEC_{oral,predator} = PEC_{water} \cdot BCF_{fish} \cdot BMF \quad (76)$$

Explanation of symbols

$PEC_{oral,predator}$	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 22

The BMF is defined as the relative concentration in a predatory animal compared to the concentration in its prey ($BMF = C_{predator}/C_{prey}$). 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 PEC_{local} 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 PEC_{local}. However, using $PEC_{regional}$ may have the opposite effect, as there may be large areas in the 200 x 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 PEC_{local}) and 50 % of the diet comes from a regional area (represented by the $PEC_{regional}$) 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 24 should be used. By establishing these factors it is assumed that a relationship exists between the BMF, the BCF and the log K_{ow} (for further explanation, see Section 4.3.3 of this Guidance on marine risk assessment). The recommended BCF triggers take into account more realistically the potential for metabolism in biota. Due to

this the use of measured BCF values as a trigger would take precedence over a trigger based on log K_{ow}.

Table 24: 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 ($PNEC_{oral}$)

Only toxicity studies reporting on dietary and oral exposure are relevant because 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 manifested 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.

The results of mammalian repeated-dose toxicity tests and data for birds (e.g. OECD test 205 (1984h): LC_{50}, 5-day acute avian dietary study or OECD test 206 (1984i): chronic) are used to assess secondary poisoning effects. Extrapolation from such test results gives a predicted no-effect concentration in food ($PNEC_{oral}$) that should be protective to other mammalian and avian species. Nevertheless, it should be considered that information from the dietary toxicity tests could be used on a case-by-case basis in higher-tier assessments when appropriate. This risk assessment scheme does not routinely use output from the LC_{50} study (EFSA 2008, Risk Assessment for Birds and Mammals).

Acute lethal doses LD_{50} (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:

$$NOEC_{bird} = NOAEL_{bird} \cdot CONV_{bird} \quad (77)$$

$$NOEC_{mammal,food\_chr} = NOAEL_{mammal,oral\_chr} \cdot CONV_{mammal} \quad (78)$$

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 23

$CONV_{mammal}$	conversion factor from NOAEL to NOEC	(kg bw·d·kg_{food}^{-1})	Table 23

Conversion factors (body weight/daily food intake ratio) for laboratory animals are presented in Table 25.

Table 25: 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 $PNEC_{oral}$ is ultimately derived from the toxicity data (food basis) applying an assessment factor. In formula:

$$PNEC_{oral} = \frac{TOX_{oral}}{AF_{oral}} \qquad (79)$$

Explanation of symbols

$PNEC_{oral}$	PNEC for secondary poisoning of birds and mammals	[in $kg \cdot kg_{food}^{-1}$]	
AF_{oral}	assessment factor applied in extrapolation of PNEC	[-]	Table 24
TOX_{oral}	either $LC_{50\ bird}$, $NOEC_{bird}$ or $NOEC_{mammal,\ food,\ chr}$	[in $kg \cdot kg_{food}^{-1}$]	

The assessment factor (AF_{oral}) 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 25 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 AF_{oral} 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 26.

Table 26: Assessment factors for extrapolation of mammalian and bird toxicity data

TOXoral	Duration of test	AForal
$LC_{50\ bird}$	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.
It is highly unlikely that sufficient avian toxicity data will be available for any substance to allow a species sensitivity distribution to be developed (i.e. an insufficient number of species will have been tested in long-term tests), so this is not considered further.

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.

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 $PNEC_{oral}$ is derived in the same way as for the aquatic route (see Section 3.8.3.5 of this Guidance). 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 $PEC_{oral,\ predator}$ is calculated as:

$$PEC_{oral,\ predator} = C_{earthworm} \quad (80)$$

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 PEC_{local} 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 of this Guidance). The same scenario is used as for the aquatic food chain (see Section 3.8.3.4 of this Guidance): i.e. 50 % of the diet comes from PEC_{local} and 50 % from $PEC_{regional}$.

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):

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} \cdot W_{earthworm} + C_{soil} \cdot W_{gut}}{W_{earthworm} + W_{gut}} \quad (81)$$

Explanation of symbols

$PEC_{oral,predator}$	Predicted Environmental Concentration in food	[mg·kg$_{wet\ earthworm}^{-1}$]
$BCF_{earthworm}$	bioconcentration factor for earthworms on wet weight basis	[L·kg$_{wet\ earthworm}^{-1}$]
$C_{earthworm}$	concentration in earthworm on wet weight basis	[mg·kg$_{wet\ earthworm}^{-1}$]
$C_{porewater}$	concentration in porewater	[mg·L^{-1}]
C_{soil}	concentration in soil	[mg·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:

$$W_{gut} = W_{earthworm} \cdot F_{gut} \cdot CONV_{soil} \quad (82a)$$

where:

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid} \cdot RHO_{solid}} \quad (82b)$$

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

The default wet-dry weight conversion factor for soil of **1.13** can be obtained using the default values of RHO_{soil}=1700 [$kg_{wwt} \cdot m^{-3}$], RHO_{solid}=2500 [$kg \cdot m^{-3}$] and the F_{solid} 0.6 [$m^3 \cdot m^{-3}$].

Using this equation, the concentration in a full worm can be written as:

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} + C_{soil} \cdot F_{gut} \cdot CONV_{soil}}{1 + F_{gut} \cdot CONV_{soil}} \quad (82c)$$

The BCF factors can be inserted in the above equation when measured data on bioconcentration in worms are available. 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):

$$BCF_{earthworm} = (0.84 + 0.012 K_{ow}) / RHO_{earthworm} \quad (82d)$$

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.[13]

[13] 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 log K_{ow} > 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,

Earthworms are also able to take up chemicals from food and it has been hypothesized that this process may affect accumulation at log K_{ow}>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 K_{ow} 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 K_{ow} 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 K_{ow} of the neutral species. The underlying data are however too limited to propose this approach in general for ionised chemicals.

3.9. Effects assessment for the marine compartment

3.9.1. Effects Assessment for the marine aquatic compartment

3.9.1.1. Introduction

Marine effects assessment should ideally be based upon data generated using a range of ecologically relevant seawater species (for example algae, invertebrates and fish). However, such data are not always available and, therefore, guidance is given on how marine hazard assessment can be based on available data on both freshwater and seawater organisms.

Usually there are fewer studies available for seawater species than for freshwater ones (as well as fewer test methods available for seawater species).

The sensitivity to narcotic chemicals is considered to be highly comparable between freshwater and seawater species. However, the marine environment contains key/abundant taxa that are not present in freshwater environments (e.g Echinodermata, Ctenophora and Cephalopoda) Given the greater species diversity in the marine environment, compared to freshwaters, including the presence of a number of taxa that occur only in the marine environment, a broader distribution of sensitivities of species, and thus a higher uncertainty in extrapolation is needed. Table 27 describes the assessment factors for marine hazard assessment, which includes a factor of 10,000 for assessments based on data from tests with the three standard freshwater species.

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 active 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)[14].

Where there is a need to assess the potential impact of substances entering estuarine and seawaters, any hazard or risk assessment should ideally be based upon data generated

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).

[14] 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 seawater (estuarine/marine) species accounted for 341 entries (15.5%).

using a range of ecologically relevant seawater species (for example algae, invertebrates and fish). This is particularly important given the greater diversity of species (particularly invertebrates) present in seawaters, relative to freshwaters. 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.

Due to these facts, the effects assessment must use, where possible, data relevant to the marine environment. 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 seawater 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 seawaters, 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.

3.9.1.2. Evaluation of data

It has been recognised for many years that there is a wider diversity of taxonomic groups (particularly invertebrates) in seawaters compared to freshwaters and that many groups are only found in seawater (see Russell and Yonge, 1928; Tait, 1978). Moss (1988) stated that 56 phyla were present in seawater compared to 41 in freshwaters. No phyla are confined to freshwaters only while 15 phyla are found only in seawater. 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 seawater biota - at least for the usual aquatic taxa (i.e., fish, crustacea, algae). No marked difference in sensitivity between freshwater and seawater 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;

The use of freshwater acute effects data *in lieu* of or in addition to seawater effects data for risk assessment purposes is not contra-indicated by the empirical data reviewed. 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. Under such circumstances, PNEC values should be derived from the most sensitive endpoint regardless of the medium. However, the use of pooled data is not recommended if there is data that shows that the species sensitivity between freshwater and marine organisms is above a factor of 10, when considering small datasets. With larger datasets, statistical testing is recommended, showing that there are no major differences in sensitivities amongst freshwater and seawater toxicity tests.

Nevertheless, toxicity data for freshwater and seawater species for metals should not be pooled *a priori* since metal speciation in different environments may greatly influence bioavailability. Only when statistical comparison shows that there is no difference in sensitivity, the datasets for metals may be pooled. Note that this may differ per taxon.

Infobox 13: Use of freshwater data for the derivation of a PNEC for marine systems

For organic compounds, the improvement of ecotoxicity data through the pooling of marine and aquatic freshwater ecotoxicity data is possible for $PNEC_{water}$ and $PNEC_{seawater}$. Pooling of available marine and freshwater ecotoxicity data for derivation of the freshwater PNEC is possible as long as the species sensitivity between freshwater and marine organisms is within a factor of 10. For larger datasets statistical testing showing no major differences in sensitivities amongst freshwater and seawater toxicity tests should if needed to consider the pooling of data.

Note that in the event of pooling of toxicity data, the assessment factor table for the marine water compartment still applies to the pooled dataset.

For inorganic compounds, the datasets for freshwater and seawater may be pooled only when statistical comparison shows that there is no difference in sensitivity, given the effects that different environments may have on the speciation and bioavailability of metal species.

Additional information can be found in the UK Defra funded research project "Addressing interspecific variation in sensitivity and the potential to reduce this in ecotoxicological risk assessments". The project addressed the issue of differences in toxicity between marine and freshwater aquatic invertebrates:

http://randd.defra.gov.uk/Default.aspx?Menu=Menu&Module=More&Location=None&Completed=0&ProjectID=9596#RelatedDocuments

3.9.1.3. Derivation of PNEC

The greater species diversity in the marine environment, compared to freshwaters (see Appendix 5), 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-taxon 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 seawater algae, crustaceans and fish is available a higher assessment factor than that for the derivation of $PNEC_{seawater}$ 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 seawater species and the issue of differences in diversity in freshwaters and seawaters. 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 $L(E)C_{50}$ 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 27 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.

Even when based on the same set of data, the $PNEC_{seawater}$ may differ from the $PNEC_{water}$.

Where data are available for additional marine taxonomic groups, the uncertainties are reduced and so the magnitude of the AF applied to a data set can be lowered (Table 27)

Data from studies with marine test organisms other than algae, crustaceans and fish, and/or having a life form or feeding strategy differing from that of algae, crustaceans or fish can be accepted as additional marine taxonomic groups and will allow a reduction in the AF applied (provided that the toxicity data are reliable and relevant). Marine species from taxa other than algae, crustaceans and fish include:

- Macrophyta. e.g. Sea grass (Zosteraceae)
- Mollusca. e.g. *Mytilus edulis, Mytulis galloprovincialis*.
- Rotifers. e.g. *Brachyonus plicatilis*.
- Hydroids (e.g. hydroids: *Cordylophora caspia, Eirene viridula*);
- Annelida. e.g. *Neanthes arenaceodentata*.

In addition, marine organisms that belong to the taxa algae, crustaceans or fish but have a different life form or feeding strategy than the representatives in the freshwater toxicity dataset can be considered additional marine taxonomic groups and may also allow a decrease in the AF:

- Macro-algae. e.g. Enteromorpha sp., Fucus sp and Champia sp.
- Crustaceans (including crabs) are found in both freshwater and seawater.

However, crabs, for example, have a life form and feeding strategy very much different from Daphnia sp., which is the test organism which is nearly always present in the freshwater toxicity data set, or other common freshwater crustaceans. Thus, such species can be used to reduce the AF where other crustaceans may not. Examples of crabs used in toxicity tests include *Cancer magister*, *Cancer pagurus*, *Carcinus maenas* and *Cancer anthonyi*.

Table 27: Assessment factors proposed for deriving PNECseawater for different data sets

Data set	Assessment factor
Lowest short-term L(E)C_{50} from freshwater or seawater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10,000 [a)]
Lowest short-term L(E)C_{50} from freshwater or seawater 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/EC_{10} (from freshwater or seawater crustacean reproduction or fish growth studies)	1000 [b)]
Two long-term NOEC/EC_{10} from freshwater or seawater species representing two trophic levels (algae and/or crustaceans and/or fish)	500 [c)]
Lowest long-term NOEC/EC_{10}s from three freshwater or seawater species (normally algae and/or crustaceans and/or fish) representing three trophic levels	100 [d)]
Two long-term NOEC/EC_{10}s from freshwater or seawater 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 NOEC/EC_{10}s from three freshwater or seawater species (normally algae and/or crustaceans and/or fish) representing three trophic levels + two long-term NOEC/EC_{10}s from additional marine taxonomic groups (e.g. echinoderms, molluscs)	10

Notes on Table 27:
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 of this

Guidance, under no circumstances a factor lower than 1000 should be used in deriving a $PNEC_{seawater}$ 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 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).

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 seawater crustacean or fish) if this NOEC was generated for the taxonomic group showing the lowest $L(E)C_{50}$ in the short-term algal, crustacean or fish tests.

If the only available long-term $NOEC/EC_{10}$ is from a species which does not have the lowest $L(E)C_{50}$ 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 $NOEC/EC_{10}$s covering two trophic levels (freshwater or seawater algae and/or crustacean and/or fish) when such NOECs have not been generated for the species showing the lowest $L(E)C_{50}$ of the short-term tests.

This should not apply in cases where the acutely most sensitive species has an $L(E)C_{50}$-value lower than the lowest $NOEC/EC_{10}$ value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest $L(E)C_{50}$ of the short-term tests.

c): An assessment factor of 500 applies to the lowest of two $NOEC/EC_{10}$s covering two trophic levels (freshwater or seawater algae and/or crustacean and/or fish) when such NOECs have been generated covering those trophic levels showing the lowest $L(E)C_{50}$ 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 $NOEC/EC_{10}$ 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 $NOEC/EC_{10}$ 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 $NOEC/EC_{10}$s 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 $L(E)C_{50}$ in short-term tests. This should, however, not apply in the case where the acutely most sensitive species has an $L(E)C_{50}$ value lower than the lowest $NOEC/EC_{10}$ value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest $L(E)C_{50}$ in the short-term tests.

d): An assessment factor of 100 will be applied when longer-term toxicity NOEC/EC_{10}s are available from three freshwater or seawater 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 NOEC/EC_{10}s 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. For instance, the availability of mesocosm studies or (semi-) field data that reflect the proposed pattern of exposure might be used for decrasing the factor of 10. Howeer, the data needs to be reviewed on a case-by-case basis (see Appendix 8).

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 of this Guidance.

3.9.2. Effects assessment for the sediment compartment

3.9.2.1. 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 seawater sediment constitutes an important compartment of marine ecosystems it may be important to perform an effects assessment for the seawater sediment compartment for those substances.

In principle, the same strategy as applied to freshwater sediment is recommended (see Section 3.5 of this Guidance) for the effects assessment of seawater 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 seawater 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 seawater 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 3.9.1.2 of this Guidance 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 seawater effects data is acceptable for risk assessment purposes. Although it is not sure that this also applies to sea- and freshwater sediment data, it is nevertheless recommended to use pooled sea- and freshwater sediment toxicity data for effect assessment for the sediment compartment. However, when sufficient data for ecologically relevant seawater species are available lower assessment factors can be applied.

3.9.2.2. 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, seawater sediment effects assessment is necessary for substances that are known to be persistent in seawater, 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 substances the number of toxicity data on benthic and sediment 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_{seased} can be determined on the basis of a measured concentration of the substance in water that is independent of the value of the K_{oc}. 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 K_{oc} or log K_{ow} value as that used to predict the $PNEC_{seased}$. 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 seawater 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 K_{ow} up to 5. For substances with a log K_{ow} > 5 (or with a corresponding K_{oc}), 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 of this Guidance).

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

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 $PNEC_{seased}$ 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 $PNEC_{seased}$ should be used for the risk characterisation.
3. where long-term toxicity data are available for benthic freshwater organisms. Under this circumstance the $PNEC_{seased}$ is calculated using assessment factors for long-term tests. This approach is explained in Section 3.9.2.4 of this Guidance.

4. where long-term toxicity data are available for benthic freshwater *and* a minimum of two marine organisms. Under these circumstances a $PNEC_{seased}$ is calculated using the lower assessment factors that are associated with data obtained from long-term tests. A $PNEC_{seased}$ obtained 3.9.2.4 of this Guidance.

Table 21 in Section 3.5.2 of this Guidance 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 seawater sediment while for whole seawater 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 seawater sediments. If not there are likely to be concerns regarding the relative bioavailability of a substance in the different sediments.

3.9.2.3. Calculations of PNEC for seawater sediment using equilibrium partitioning

In the absence of any ecotoxicological data for sediment-dwelling organisms, but with measured data to predict the PEC_{seased}, the $PNEC_{seased}$ may provisionally be calculated using the equilibrium partitioning method. This method uses the $PNEC_{seawater}$ 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 of this Guidance. 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

$PNEC_{seawater}$	Predicted No Effect Concentration in seawater	$[mg \cdot l^{-1}]$	
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)
$PNEC_{seased}$	Predicted No Effect Concentration in seawater sediment	$[mg \cdot kg^{-1}]$	

In Section 3.5.2 of this Guidance a remark is made with respect to the calculation of $PNEC_{seased}$ 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 K_{ow} greater than 3. Direct uptake from seawater 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 seawater sediment that the proportion of the total dose taken up through intake of sediment particles remains low for chemicals with a log K_{ow} 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 K_{ow} greater than 5 (or with a corresponding $K_{p,\ sed}$) 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 > 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.

3.9.2.4. Calculation of PNEC for seawater sediment using assessment factors

If results from whole-sediment tests with benthic organisms are available the $PNEC_{seased}$ 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 of this Guidance). Table 28 describes the assessment factors for seawater sediment hazard assessment when only short-term sediment toxicity tests are available, and Table 29 defines the assessment factors when at least one long-term sediment toxicity test is available.

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 $PNEC_{seased}$ should also be calculated from the $PNEC_{sea\text{-}water}$ 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 seawater tests) is available then an assessment factor of 1000 is applicable. Once again a $PNEC_{seased}$ should also be calculated from the $PNEC_{seawater}$ 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 $PNEC_{seased}$ is derived by application of the following assessment factors to the lowest LC_{50} value from acute tests:

Table 28: Assessment factors for derivation of $PNEC_{seased}$ from short-term sediment toxicity tests

Available test results	Assessment factor	PNECseased
One acute freshwater or seawater test	10,000	Lowest of LC_{50} /10,000 and equilibrium-partitioning method
Two acute tests including a minimum of one seawater test with an organism of a sensitive taxa	1000	Lowest of LC_{50} /1000 and equilibrium-partitioning method

A $PNEC_{seased}$ is derived by application of the following assessment factors to the lowest $NOEC/EC_{10}$ value from long-term tests:

Table 29: Assessment factors for derivation of $PNEC_{seased}$ 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 seawater 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 of this Guidance) must 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 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 seawater 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 30. 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 seawater 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 30: 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 is 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) EPA 600-R-01-020 (2001) Method for Assessing the Chronic Toxicity of Marine and Estuarine Sediment-associated Contaminants with the Amphipod *Leptocheirus plumulosus.*	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

Test organism	Acute or chronic test	Duration	Endpoints	Reference	
POLYCHAETES					
Nereis/Neanthes sp Neanthes arenaceodentat akan 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.
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 row above. Changes in feeding rate have consequences for sediment communities. SOP [1)] available, equipment and test species commercially available. OSPAR ringtested
ECHINODERMES					
	acute/ subchronic	14 d	Survival	Stronkhorst (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

3.9.3. Assessment of secondary poisoning

3.9.3.1. 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 K_{ow} typically > 4.5 or BCF > 500) and are also resistant to biotransformation in animals. Biomagnification (increased food chain accumulation) of such chemicals 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 $PEC_{seawater}$ 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.

3.9.3.2. Assessment of bioaccumulation and secondary poisoning

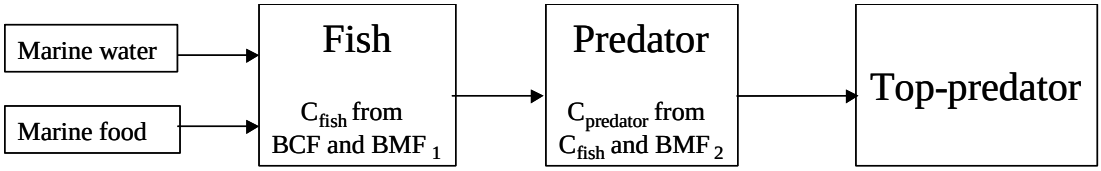
The assessment scheme

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 seawater phase, marine food, marine fish and two separate levels of

predators. This food chain is visualised in Figure 17. 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 ($PNEC_{oral,\ predator}$). 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 ($PNEC_{oral,\ top\ predator}$). 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 PEC_{oral} and $PNEC_{oral}$ is not based on internal concentrations but on intake rates.

Figure 17: 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:

$$PEC_{oral,predator} = PEC_{seawater} \cdot BCF_{fish} \cdot BMF_1 \qquad (89)$$

$$PEC_{oral,toppredator} = PEC_{oral,predator} \cdot BMF_2 = PEC_{water} \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2 \quad (90)$$

Explanation of symbols

$PEC_{oral,\ predator}$	concentration in the food of the predator	[mg·kg^{-1}]	
$PEC_{oral,\ top\ predator}$	concentration in the food of the top predator	[mg·kg^{-1}]	
$PEC_{seawater}$	concentration in seawater	[mg·l^{-1}]	
BCF_{fish}	bioconcentration factor	[l·kg^{-1}]	eq. (73)
BMF_1	biomagnification factor in fish	[-]	Table 31
BMF_2	biomagnification factor in the predator	[-]	Table 31

The BMF used should, ideally, be based on measured values. BMFs can be derived from trophic magnification studies. Additional guidance can be found in the Water Framework Directive Technical Guidance for deriving Environmental Quality Standards, section 4.7.2.1 of this Guidance. 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 K_{ow} of the substance under defined conditions, the available data are not conclusive. Other more complex intrinsic properties of substances, than the lipophilicity (log K_{ow}), 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 K_{ow} up to 4.5 biomagnification seems generally to be low and thus BMF = 1. For higher log K_{ow} the biomagnification increases up to around log K_{ow} 7 and then it decreases again to be low around log K_{ow} 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 31 are suggested. If a BCF for fish is available, it is possible to use that as a trigger instead of log K_{ow}. The BCF triggers recommended are less conservative than the log K_{ow} 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 K_{ow}.

Table 31: Default BMF values for organic substances with different log K_{ow} or BCF in fish

log Kow	BCF (fish)	BMF1	BMF2
< 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 K_{ow} 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 K_{ow}, 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 PEC_{oral} for the predators this implies the following:

$$PEC_{seawater} = 0.5 \cdot \left(PEClocal_{seawater,ann} + PECregiond_{seawater} \right) \quad (91)$$

When $PEC_{seawater}$ is substituted in equation 89 this results in the following equation:

$$PEC_{oral,predator} = \left(PEClocal_{seawater,ann} + PECregiond_{seawater} \right) \cdot 0.5 \cdot BCF_{fish} \cdot BMF_1 \quad (92)$$

Explanation of symbols

$PEC_{oral,\ predator}$	concentration in the food of the predator	[mg·kg^{-1}]	
$PEC_{seawater}$	concentration in seawater	[mg·l^{-1}]	
BCF_{fish}	bioconcentration factor	[l·kg^{-1}]	eq. (73)
BMF_1	biomagnification factor in fish	[-]	Table 31
$PEC_{regional,seawater}$	predicted environmental concentration in the region	[mg·l^{-1}]	
$PEC_{local,\ seawater,ann}$	annual average predicted environmental concentration	[mg·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 ($PEC_{oral,\ top\ predator}$) this implies:

$$PEC_{water} = 0.1 \cdot PEClocal_{seawater,ann} + 0.9 \cdot PECregiond_{seawater} \quad (93)$$

When PEC_{water} is substituted in equation 90 this results in the following equation:

$$PEC_{oral,top-predator} = \left(0.1 \cdot PEClocal_{seawater,ann} + 0.9 \cdot PECregiond_{seawater}\right) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2 \quad (94)$$

Derivation of the $PNEC_{oral}$ values

In the derivation of the $PNEC_{oral}$ 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 of this Guidance).

3.9.3.3. 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 K_{ow} 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 $PNEC_{oral}$ could be considered, i.e. to require a long-term feeding study with laboratory mammals or birds to derive a more realistic $NOEC_{oral}$ 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.

3.10. Effect assessment for rapidly degrading substances

3.10.1. Introduction

This chapter was provided as a proposal for harmonisation in the use of the time weighted average (TWA) and other available approaches to define effect data endpoints in aquatic and soil studies where the test concentrations cannot be maintained throughout the test.

Much of the available guidance on environmental testing, exposure and risk assessment strategies concentrates on the issue of persistence and does not sufficiently addresses the issue of rapidly degrading substances. This is of particular concern for risk assessors and experimenters when testing the effects of non-persistent or rapidly degrading substances in tests where method modifications such as flow-through or static-renewal are not practical i.e. algal, sediment and soil ecotoxicological tests. Furthermore, several biocidal uses result in a continuous or semi-continuous long-term emision of such non-persistent substances. Therefore, additional guidance on how and when to assess the no effect concentration is desirable for substances in aquatic and soil studies where the concentrations cannot be maintained throughout the exposure period of the test.

Special care should be taken in the evaluation of such rapidly degrading substances that this rapid degradation is sufficiently considered for a balanced risk characterisation (PEC/PNEC). If a substance shows a rapid degradation, this is normally already considered for the exposure estimation, leading to a correspondingly lower PEC. To use nominal or initial measured concentrations on the effects side instead of (mean) measured concentrations would lead to an underestimation of the risk for the environment. This means, there is no disadvantage of degradable substances by using the approach outlined below but it ensures a balanced risk assessment. However, the reverse situation often occurs in the risk assessment for the terrestrial compartment. $PNEC_{soil}$ is often based on studies with initial soil concentrations, i.e. exposure in tests is not corrected for degradation. Therefore, for the soil compartment the PEC_{soil} should not be corrected for degradation, given that if the PEC_{soil} was corrected but the test soil concentrations were not, that would lead to an underestimated risk quotient ($PEC_{soil}/PNEC_{soil}$).

3.10.2. Proposal for a hamonised assessment

The following proposals provide a basis for a consistent approach to assess ecotoxicological endpoints for active substances that rapidly degrade in the test system. These proposals only apply to robust tests conducted following standard guidelines where the substances tested cannot be maintained throughout the test even using techniques such as semi-static or flow-through. These rules cannot be applied for endpoints to be derived from unacceptable or poor quality studies.

The proposals are based on the OECD Guidance Document No. 23 (2000) on aquatic toxicity testing of difficult substances and mixtures, with additional consideration of the potential exposure patterns for biocidal products. These approaches are to be used for the determination of the mean exposure concentration in acute or chronic tests where a substance can be shown to degrade significantly over the course of a test (< 80 % of nominal reported).

The following options are available:

(a) If measured concentrations at test start and end are available for all concentration levels tested or for the concentration levels that are close to the derived effect value, the mean (geometric) measured concentrations may be calculated. It is proposed to use the square root geometric mean formula for the calculation of the geometric mean.

(b) Where a measured concentration at the end of the exposure period is absent or where it indicates that the substance is not detected, the validity of the test should first be reconfirmed. If analytical data indicates that the substance could not be:

   i. detected by the end of the study, the final concentration may be taken as the limit of detection (LOD) and the mean (geometric) measured concentrations can be calculated as in (a).

   ii. quantified by the end of the study, the final concentration may be taken as half the limit of quantification (LOQ/2) for the method and the mean (geometric) measured concentrations can be calculated as in (a).

Since there may be various methods for determining the above parameters, the method selected to determine mean measured concentrations should be made explicit in the reporting of test results. This is because the concentration might not be measurable.

(Options (a) and (b) are taken directly from the OECD GD on Difficult Substances) and apply mainly to aquatic studies including algae. Aquatic studies for rapidly degrading substances performed without any analytical monitoring have to be regarded as invalid as a deviation of more than 20 % from the nominal concentration is expected.

If analytical monitoring was also performed in soil studies the approaches (a) and (b) may also apply to these studies.

(c) If no analytical data of the (final) concentrations are available, the mean measured concentrations is calculated using the:

TWA approach as detailed for Plant Protection Products (Regulation (EC) No 1107/2009).

$$C = C_0 \cdot f_{twa} \quad (95)$$

Explanation of symbols

C_0	Initial concentration at test start	
f_{twa}	Time-weighted-average factor	$(1-e^{-kt})/kt$
k	$ln2/DT_{50}$ (velocity constant)	
t	Test duration	

The calculation of a TWA concentration for static soil (or sediment) tests is only used for substances that do not degrade too fast in the test system as this would lead to unrealistically low effect values. The following cases are proposed:

1) Substances with an expected degradation half-life of < 2 d:

It is unlikely that a sensitive endpoint from a static soil or sediment study (test duration normally in the range of 14 – 21 d) can be derived, as the use of TWA would result in unrealistically low effect values. For such substances, any toxicity observed in the tests might predominantly be caused by one ore more degradation product(s). The use of the nominal or initial measured concentration is nevertheless justified if the PNEC derived from these tests is compared with the initial PEC without considering degradation, if the true exposure pattern due to the biocidal use is similar to that of the effect test method. In addition, a risk assessment for the relevant metabolites would need to be performed. If the environmental exposure is due to a semi-continuous pattern, it is proposed to sum, in the exposure assessment, the PEC of the active substance and the PEC of the metabolite(s), then thisPEC would be compared with the PNEC based on nominal or initial measured concentrations.

2) Substances with an expected degradation half-life of ≥ 2 d:

Endpoints from acute and chronic studies (soil/sediment) should be derived using TWA. The risk assessment should also consider the relevant metabolite(s). This approach should also be applied for substances with a half-life < 2 d that have a continuous release. It is important, however, that when the PNEC for soil/sediment studies is derived using TWA method, the predicted environmental concentration (PEC) should also reflect a time weighted average concentration.

The half-life to be used for the estimation of the mean concentration should be selected from the available studies based on expert judgement. It should be corrected to the standard test temperature (20 °C). However, the calculation of TWA is only valid when the degradation pattern follows first order kinetics. It has to be considered that the application of half-lives from soil degradation studies performed with real soil to ecotoxicological studies performed with artificial soil represents a worst-case situation as the degradation of the test substance in the artificial soil is likely lower than in real soils due to the lower microbial activity. However, as normally no other information on degradation in soil is available, it is recommended to use these half-lives as first approach. If a risk is identified based on the half-lives from soil degradation studies, a new effect test could be performed with chemical analysis of the test substance concentration in the test system at least at

test start and test end; for long-term test or if fast degradation is expected additional measurements between test start and end (in separate analytical vessels) are advisable.

If for a substance there is information on the mode of action from which it can be concluded that effects are only expected to be acute (e.g. oxidising substances), the initial concentrations can be used for the effects assessment and compared with the initial PEC for the risk characterisation. Examples for such substances are hydrogenperoxide or hypochlorite. However, for most biocidal active substances this information is not available. It has to be considered that the information available on the mode of action from efficacy tests cannot automatically be used to conclude on the mode of action in ecotoxicity tests, as a substance can act by different mode of actions (e.g. herbicidal and insecticidal activity) or the available information does not allow a statement on acute versus chronic effects.

3.11. Assessment of exclusion criteria

Active substances cannot be approved if they fulfil the exclusion critera according to Article 5(1) of the BPR:

1. are Carcinogens category 1A or 1B, Mutagens category 1A or 1B, or toxic for Reproduction category 1A or 1B,
2. have endocrine-disrupting properties, or
3. are persistent, bioaccumulative and toxic (PBT) or very persistent and very bioaccumulative (vPvB)

Derogations apply according to Article 5(2) of the BPR if the risk is negligible, the substance is essential to control a serious danger to human or animal health or to the environment, or the non-approval will have disproportionate negative impact for society.

Ad 2): For the assessment of endocrine disrupting properties, guidance is currently under preparation.

Ad 3): PBT substances are substances that are persistent, bioaccumulative and toxic, while vPvB substances are characterised by a particular high persistence in combination with a high tendency to bio-accumulate, but not necessarily proven toxicity. These properties are defined by the criteria laid down in section 1 of Annex XIII of REACH (Criteria for the Identification of Persistent, Bioaccumulative and Toxic Substances, and very Persistent and very Bioaccumulative Substances, henceforth "the PBT and vPvB criteria").

Experience with PBT/vPvB substances has shown that they can give rise to specific concerns that due to their potential to accumulate in parts of the environment and/or biota, and the effects of such accumulation are unpredictable in the long-term; such accumulation is practically difficult to reverse as cessation of emission will not necessarily result in a reduction in the substances concentration.

Furthermore, PBT or vPvB substances may have the potential to contaminate remote areas that should be protected from further contamination by hazardous substances resulting from human activity as the intrinsic value of pristine environments should be protected.

These specific concerns occur particularly with substances that can be shown both to persist for long periods and to bioaccumulate in biota and which can give rise to toxic effects after a longer time and over a greater spatial scale than chemicals without these properties. These effects may be difficult to detect at an early stage because of long-term exposures at normally low concentration levels and long life-cycles of species at the top of the food chain. In case of vPvB chemicals, there is concern that even if no toxicity is demonstrated in laboratory testing, long-term effects might be possible since high and unpredictable levels may be reached in human or the environment over extended time periods.

Guidance on how to conduct a PBT assessment as well as the screening criteria and information for the identification of PBT/vPvB properties on substances can be found in the *Guidance on information requirements and chemical safety assessment Chapter R.11: PBT Assessment* according to the criteria stated in Annex XIII of REACH. Nevertheless, the information requirement for the BPR may differ than that required for REACH.

Moreover, Article 2(3) of the BPR outlines the Directives and Regulations to which the BPR must also apply. The provisions for substance under these Directives and Regulations should also be considered for the assessment of exclusion criteria of biocidal active substances.

4. Risk Characterisation

According to BPR Annex VI, the risk characterisation for the environment considers the estimation of the incidence and severity of the adverse effects likely to occur in environmental compartments due to actual or predicted exposure to any active substance or substance of concern in a biocidal product.

For any given environmental compartment, the risk characterisation must, as far as possible, entail comparison of the PEC with the PNEC so that a PEC/PNEC ratio may be derived. If it has not been possible to derive a PEC/PNEC ratio, the risk characterisation must entail a qualitative evaluation of the likelihood that an effect is occurring under the current conditions of exposure or will occur under the expected conditions of exposure.

4.1. 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 of this Guidance:

Inland environmental compartments:

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

Marine environmental compartments:

- aquatic ecosystem (inlcuding seawater sediment);
- top predators.

A list of the different PEC/PNEC ratios that should be considered for the inland and marine environments is given in Tables 31 and 32, respectively.

Table 32: Overview of PEC/PNEC ratios considered for fresh-/surface water risk assessment*

Local	Regional
$PEC_{local,\ water}/PNEC_{water}$	$PEC_{regional,\ water}/PNEC_{water}$
$PEC_{local,\ sediment}/PNEC_{ediment}$	$PEC_{regional,\ sediment}/PNEC_{sediment}$
$PEC_{local,\ soil}/PNEC_{soil}$	$PEC_{regional,\ agr.soil}/PNEC_{soil}$
$PEC_{stp}/PNEC_{stp}$	
$(0.5 \cdot PEC_{local,\ oral,\ fish} + 0.5 \cdot PEC_{regional,\ oral,\ fish})/PNEC_{oral}$	
$(0.5 \cdot PEC_{local,\ oral,\ worm} + 0.5 \cdot PEC_{regional,\ oral,\ worm})/PNEC_{oral}$	

* 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
$PEC_{local,\ seawater}/PNEC_{seawater}$	$PEC_{regional,\ seawater}/PNEC_{seawater}$
$PEC_{local,\ seased}/PNEC_{seased}$	$PEC_{regional,\ seased}/PNEC_{seased}$
$[(PEC_{local,\ seawater,ann} + PEC_{regional,\ seawater}) \cdot 0.5 \cdot BCF_{fish} \cdot BMF_1]/PNEC_{oral,\ predator}$	
$[(0.1 \cdot PEC_{local,\ seawater,ann} + 0.9 \cdot PEC_{regional,\ seawater}) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2]/PNEC_{oral,\ top\ predator}$	

* 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 4.4 of this Guidance.

Infobox 14: Sediment risk assessment for metabolites / Risk assessment for metabolites in general

Concerning the risk assessment of metabolites a difference is made between:
Major metabolite: see Infobox 1
Minor metabolite: metabolites that are no major metabolites
Ecotoxicologically relevant metabolite: any minor or major

If there is any reason for concern, a risk assessment also needs to be performed for those ecotoxicologically relevant metabolites which are **minor** metabolites.

Sediment risk assessment for metabolites

Substances with a K_{oc} value less than 500 or with a corresponding adsorption or binding behaviour triggered by the lipophilicity (e.g. log K_{ow}) are not likely to adsorb to sediment and to avoid extensive testing of chemicals it should not trigger a sediment effects test. This approach should be followed with the exception of cases where an influence on sediment may be observed. In these cases, a sediment risk assessment for metabolites is needed.

4.2. General premises for risk characterisation

In general, the risk characterisation phase is carried out along the following steps:

- 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. The risk characterisation should describe the assumptions and uncertainties in a transparent manner.

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.

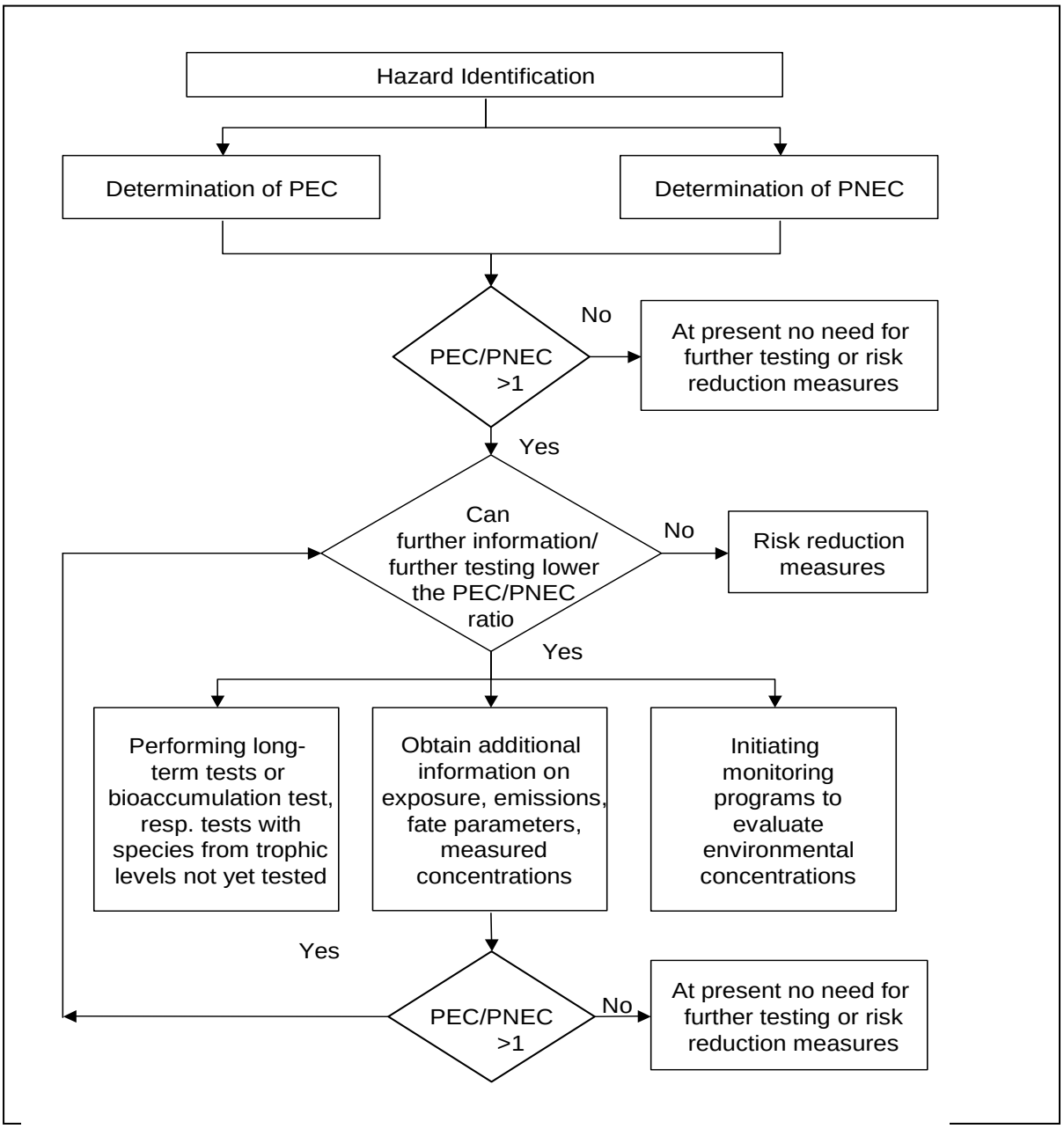
For the air compartment usually only a qualitative assessment of abiotic effects is carried out. If there are indications that one or more of these effects occur for a given substance, expert knowledge should be consulted or the substance be handed over to the relevant international group, e.g. to the 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 PEC_{oral} with the $PNEC_{oral}$ in accordance with the procedure described in Sections 3.8 and 3.9.3. If the ratio PEC_{oral} / $PNEC_{oral}$ is greater than one and a refinement of the PEC_{oral} or the $PNEC_{oral}$ 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 $PNEC_{stp}$. 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 18: 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 risk reduction and mitigation measures are needed for the substance.

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. 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 Guidance on information requirements and chemical safety assessment. *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*.

4.3. Specific premises for the risk characterisation for biocides

The environmental risk characterisation for biocidal active substances in the context of BPR Annex VI involves i.a. the comparison of PEC and PNEC values for relevant environmental compartments as well as for non-target organisms. 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 the Union List of Authorised Active Substances of the Regulation (in the following referred to as Union List);
- the substance may be considered for inclusion in the Union List.

Infobox 15: Tiered approach

The risk to environmental compartment follows in general a tiered approach. The first tier is a general conservative evaluation of the behaviour and toxicity of the substance in the environment. It is in general based on model data regarding exposure, laboratory toxicology studies and for example, the equilibrium partitioning for certain PNEC derivations.

If the trigger values of the first tier of the evaluation are not met, the applicant is offered the opportunity to submit additional data for conducting a refined risk evaluation (higher tier). In general this includes additional chronic studies (aquatic and soil) and/or more realistic exposure data. Alternatively, the applicant can choose for risk reduction measures, but the applicant must prove that these measures are in practice realistic, effective and reduce the risk(s) to acceptable levels.

The decision on inclusion in the Union List of the BPR also depends on other criteria regarding, e.g., other unacceptable effects and efficacy (cf. Regulation 528/2012 and the Practical guide chapters in relation to Active Substances). The inclusion may, where appropriate, be subject to certain requirements and conditions for use.

Additional to these main conclusions, some substances included in the Union List may be candidates for substitution (Article 10 of Regulation 528/2012). See also Section 4.7 of this Guidance.

If the PEC/PNEC ratio is > 1 the Competent Authority must 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 the Union List at all.

Finally, if a quantitative risk characterisation cannot be conducted, a qualitative risk characterisation should be conducted, cf. below.

For in-situ generated active substances, the risk assessment includes also the possible risks from the precursor(s).

Infobox 16: Risk assessment and data requirements for bees and beneficial arthropods

At the moment no method is available for biocides on how to perform the risk assessment for bees and non-target arthropods. The methods applied under the pesticides EU framework are not directly applicable. However, if tests on bees or non-target arthropods are performed, or are available, these could be use for a qualitative risk assessment if exposure pattern is comparable. Based on the outcome of these tests risk mitigation measures can be considered.

If tests on non-target arthropods have to be performed, tests on soil dwelling organisms like springtails are preferred.

With respect to the data requirement for bees and non-target arthropods (NTA) tests are required only in case of large scale-outdoor applications like fogging (e.g. products against mosquitoes for human health reasons).

Additionally, for neonicotinoid substances or other insecticide substances with high toxicity to bees, exposure to bees should also be quantified. When no data is available, a qualitative assessment should be performed.

4.4. 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. Situations for which this might be the case include: the assessment of risks for remote marine areas, substances where either PEC or PNEC cannot be properly calculated, or when expert judgement suggests that the use of certain molecules will lead to negligible emissions (e.g., the use of ethanol, hydrogen peroxide or peracetic acid on surfaces). In these cases, the risk characterisation must entail a qualitative evaluation of the likelihood that an effect will occur under the expected conditions of exposure.

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 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 K_{ow} > 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. K_d 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 K_{ow} > 3 (or BCF > 100) and a PEC_{local} or $PEC_{regional}$ > $1/100^{th}$ 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 log K_{ow} is not a good indicator of bioconcentration, or where there are other indications of a potential to bioconcentrate (see Section 3.8 of this Guidance), a case-by-case assessment of the presumable long-term effects will be necessary.

4.5. Risk characterisations for specific substance groups

4.5.1. Risk characterisations for metals and metal compounds

4.5.1.1. Introduction

This section gives a general outline on how to perform risk assessments for metals using the methods that are available for risk assessment of active substances 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 $ZnSO_4$, $ZnCl_2$. 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 Section 3 of this Guidance. 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. 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[15].

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).

4.5.1.2. 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,

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15 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 $[Ni] = 10 + L$.

corrosion, etc. 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.

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, PEC_{local}, 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 K_p values will have to be used (Section 2.3.7 of this Guidance). 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 K_p 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, $PEC_{regional}$. 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 (K_p), 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 this Guidance). The same applies to the bioconcentration factors required: only experimentally determined values should be used. For soils, the K_p 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 K_p 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 19.

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 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 Council Directive 2006/11/EEC of the European Parliament and of the Council of 15 February 2006 on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community 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 K_p 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.

Figure 19: Use of multimedia fate models for metals

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.

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, e.g. 10-20 Pa. This leads to a value for $F_{ass,\ aer}$ 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 above, 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.)

   The values applied for model parameters for the regional model (Table 12), intermedia mass transfer coefficients (Table 13) and model parameters for the continental concentration (Table 14) can be used.

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 K_p 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 K_p 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, K_p values are expressed in terms of concentrations available for uptake by biota in both the aqueous and the solid phase:

$$K_p = \frac{total\ available\ concentration\ in\ solid\ phase}{concentration\ in\ aqueous\ phase} \quad (95)$$

It is of importance to be aware that equation 95 differs from the commonly used expressions for K_p 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 K_p values according to equation 95. 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 K_p 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.

4.5.1.3. 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 Section 3.2 of this Guidance. 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). 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 of this Guidance. 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 this Guidance).

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 regulates 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. From the above it is clear that it is not appropriate to apply classical concepts (e.g. use of BCF,BMF) to metals as they are applied to organic substances. At the same time, log K_{ow} values for metals and other inorganic compounds are not applicable for predicting their bioaccumulation potential and scientific judgement and/or studies are necessary.

4.5.1.4. Risk Characterisation

The risk characterisation of metals basically follows the principles set out in Section 4.2 of this Guidance. 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 is often possible to convert measured total concentrations to dissolved concentrations. For terrestrial systems this is possible by applying the appropriate K_p values.

References

Cleven RFMJ, Janus JA, Annema JA and Slooff W (eds.) (1993). Integrated Criteria Document Zinc. RIVM report No. 710401028.

Luoma SN (1983). Bioavailability of trace metals to aquatic organisms - a review. The Science of the Total Environment 28, 1-22.

Ministry of VROM (1994). Environmental Quality Objectives in the Netherlands, Den Haag, The Netherlands.

Ontwerp-uitvoeringsbesluit bij het vlaamse bodemsaneringsdecreet (24-01-1995) houdende achtergrondwaarden en bodemsaneringsnormen (document on background concentrations in Flanders, Belgium).

Parametrix Inc. (draft February 1995). Aquatic Ecotoxicity Testing of Sparingly Soluble Metals and Metal Compounds. Prepared for the Mining Association of Canada, Washington.

Ure AM, Davidson CM (eds.) (1995). Chemical Speciation in the Environment. Blackie Academic & Professional, Glasgow.

Van der Kooij LA, van de Meent D, van Leeuwen CJ, Bruggeman WA (1991). Deriving quality criteria for water and sediment from the results of aquatic toxicity test and product standards: application of the equilibrium partitioning method. Wat. Res. 25, 697-705.

Van Tilborg WJM and van Assche F (1995). Integrated Criteria Document Zinc: Industry Addendum. Projectgroep Zink BMRO-VNO, Roozendaal.

Van Wensem J, Vegter JJ, van Straalen NM (1994). Soil quality derived from critical body concentrations of metals in soil invertebrates. Appl. Soil Ecol. 1, 185-191.

Wood JM (1974). Biological cycles for toxic elements in the environment. Science 188, 1049-1052.

4.5.2. Risk characterisation for petroleum substances

4.5.2.1. Introduction

In this section 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.

4.5.2.2. 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, which can be either 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 additive:

$$\frac{PEC}{PNEC}_{whole\ substance} = \frac{PEC_A}{PNEC_A} + \frac{PEC_B}{PNEC_B} + \frac{PEC_C}{PNEC_C}\ etc. \qquad (96)$$

where: A,B,C etc. are the blocks.

This is referred to as the Hydrocarbon Block Method (HBM). Please refer also to the *Transitional Guidance on mixture toxicity assessment for biocidal products for the environmen*t (http://echa.europa.eu/documents/10162/15623299/biocides_transitional_guidance_mixture_toxicity_en.pdf), which contains more recent research and updated reflections on general mixture toxicity aspects.

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 block 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 than one petroleum substance. In principle the HBM allows to calculate 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 HBM

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, blockscan 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/EC_{50}s 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 blocksand 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 above sections and the HBM. This means that a PEC_{local} and $PEC_{regional}$ can be calculated as described in Chapter 2 of this Guidance and a PNEC can be derived as described in Chapter 3 of this Guidance.

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, the 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 should 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 identification 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 $PEC_{regional}$. It appeared that for definition of the blocks the log K_{ow} is the main parameter. This implies that blocks can be defined on equally spaced log K_{ow} 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). Please refer also to the "Transitional Guidance on mixture toxicity assessment for biocidal products for the environment" (http://echa.europa.eu/documents/10162/15623299/biocides_transitional_guidance_mixture_toxicity_en.pdf), which contains more recent research and updated reflections on general mixture toxicity aspects.

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 mainly 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 must 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 K_{ow}, 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 *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*.

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 core 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 of the TGD (2003) 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 TGD) 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 Volume V (Use of QSARs).

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 the 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 (2003). However, these QSARs can only be applied in a range of log K_{ow} from approximately 2-6. For chemicals with higher log K_{ow} 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 K_{ow} values, this may lead to unrealistic PNEC values;
- as an indication above log K_{ow} 6, a parabolic equation to derive a BCF for fish can be used (see Section 3.8.3.2 of this Guidance) in combination with the critical body burden (CBB) 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 $PEC_{regional}$.

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. 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:

1. specific blocks have PEC/PNEC values > 1 or;
2. 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 (2003) 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.

References

Adema DMM and Bos-Bakker GH (1986). The Aquatic Toxicity of Compounds that may be carried by Ships (Marpol 1973, Annex II). Progress report for 1986 from TNO to Dutch Ministry of Housing, Physical Planning and the Environment.

Adema DMM (1991). The Acute Aquatic Toxicity of Alkylbenzenes. Report from TNO to Dutch Ministry of Housing, Physical Planning and the Environment.

CONCAWE Ecology Group (1995). Environmental risk assessment of petroleum products - Hydrocarbon Block Approach. Brussel.

ECETOC (in press). The Role of Bioaccumulation in Environmental Risk Assessment: The Aquatic Environment and the Related Food Web.

EIFAC (1987). Revised Report on Combined Effects on Freshwater Fish and other Aquatic Life of Mixtures of Toxicants in Water. European Inland Fisheries Advisory Commission (EIFAC), Working party on Water Quality Criteria for European Freshwater Fish. EIFAC Technical Paper (37), Rev. 1.

EU (1995). Workshop on Environmental Risk Assessment of Petroleum Substances. 6-7 December 1994. European Commission, Joint Research Center, Institute for Health and Consumer Protection, European Chemicals Bureau (ECB), Ispra (VA), Italy.

Hermens JLM (1989). Quantitative Structure-Activity Relationships of Environmental Pollutants. In: Handbook of Environmental Chemistry, volume 2E. Hutzinger O (Ed.), Springer Verlag, Berlin, 111-162.

Sijm DTHM, Schipper M and Opperhuizen A (1992). Toxicokinetics of halogenated benzenes in fish: lethal body burden as a toxicological end point. Environ. Toxicol. Chem. 12, 1117-1127.

Verburgh et al. (1995). Criteria for Hydrocarbon Blocks as Input for Risk Assessment of Hydrocarbon Mixtures. European Commission, Joint Research Center, Institute for Health and Consumer Protection, European Chemicals Bureau (ECB), Report U11/JVtg1 of ECB, Ispra (VA), Italy.

Verhaar HJM, van Leeuwen CJ and Hermens JLM (1992). Classifying environmental pollutants. Structure-activity relationships for prediction of aquatic toxicity. Chemosphere 25(4), 471-491.

4.5.2. Risk characterisation for ionising substances

4.5.2.1. 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.

4.5.2.2. 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 K_{ow}.

The basic parameters used in the exposure assessment (log K_{ow}, 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 K_p in soil, sediment, and suspended solids need to be corrected. This can be done by using a correction factor (see footnote on page 103).

The 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 K_{ow} 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.

4.5.2.3. 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.

4.5.2.4. 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.

4.6. Risk assessment of sources not covered by the life-cycle of the substance

4.6.1. Introduction

Exposure may occur from other sources than the life-cycle of the active substance under assessment. Such sources have been referred to as "unintentional sources". Examples are substances of natural origin 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 active substance. 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 the following, some recommendations are given on how to deal with these kinds of sources.

4.6.2. Legal background

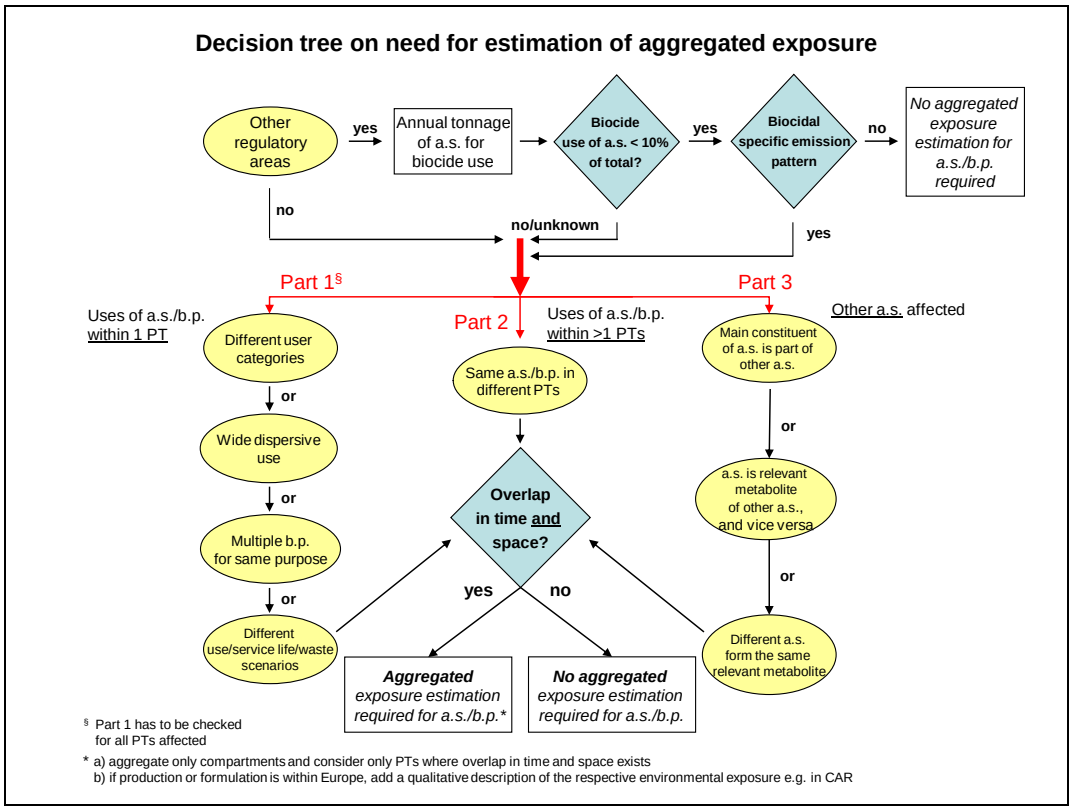
The BPR states that cumulative effects from the biocidal products containing the same active substances must be taken into account, where relevant, in the assessment of a biocidal active substance.

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 BPR (e.g. in plant protection products) and maybe regulated with another Regulation there is, at the time of the preparation of this guidance, 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.

4.7. Assessment of aggregated exposure

Guidance currently under development: to be added at a future update. The following decision scheme has been discussed:

Figure 20: Decision tree on the need for estimation of aggregated exposure



5. References

NOTE to the reader:
This list of references has been taken from TGD 2003 and wil be reviewed and revised at the first update forseen to start later this year (2015).

Ahlers J, Koch W, Lange A, Marschner A, Welter G (1992). Bewertung der Umweltgefährlichkeit von Alten Stoffen nach dem Chemikaliengesetz (ChemG). Chemikaliengesetz-Heft 10, Texte 19/92, Umweltbundesamt, Berlin.

Aldenberg T and Slob W (1993). Confidence limits for hazardous concentrations based on logistically distributed NOEC toxicity data. Ecotoxicology and Environmental Safety **25**, 48-63.

Aldenberg T and Jaworska JS (2000). Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. Ecotoxicology and Environmental Safety **46**(1), 1-18.

ASTM (1990a). Standard Guide for Conducting 10-Day Static Sediment Toxicity Tests with Marine and Estuarine Amphipods. American Society for Testing and Materials (ASTM), ASTM Standard E 1367-90, Philadelphia, PA, 1-24.

ASTM (1990b). Guide for Designing Biological Tests with Sediments. American Society for Testing and Materials (ASTM), Subcommittee Ballot, Draft #1 dated 10/19/90, Jim Dwyer, 314/875-5399, Philadelphia, PA.

ASTM (1990c). Guide for Determination of the Bioaccumulation of Sediment-Associated Contaminants by Fish. American Society for Testing and Materials (ASTM), Concurrent Subcommittee and Main Committee Ballot, Draft #2 dated 04/17/90, Mike Mac, 314/994-3331, Philadelphia, PA.

ASTM (1990d). Guide for Determination of the Bioaccumulation of Sediment-Associated Contaminants by Benthic Invertebrates. American Society for Testing and Materials (ASTM), Subcommittee Ballot, Draft #3 dated September 1990, Henry Lee, 503/867-4042, Philadelphia, PA.

ASTM (1990e). Sediment Testing Methods. American Society for Testing and Materials (ASTM), Draft #1, dated 11/06/90, Philadelphia, PA.

ASTM (1991). Standard Guide for Conducting Sediment Toxicity Tests with Freshwater Invertebrates. American Society for Testing and Materials (ASTM), ASTM Standard E 1383-90, Marcia Nelson, 314/875-5399, Philadelphia, PA, 1-20.

ASTM (1993). Standard Guide for Conducting 10-Day Static Sediment Toxicity Tests with Marine and Estuarine Amphipods. American Society for Testing and Materials (ASTM), Annual Book of Standard, Vol. 11(04), E1367-92.

ASTM (1994). Standard Guide for Conducting Sediment Toxicity Tests with Marine and Estuarine Polychaetous Annelids. American Society for Testing and Materials (ASTM), E1611-94.

Austen MC and Somerfield PJ (1997). A community level sediment bioassay applied to an estuarine heavy metal gradient. Mar. Environ. Res. **43**, 315-328.

BBA (1986). Fate of Plant Protection Agents in Soil-Degradation, Conversion and Metabolism for Simulation of the Compartment Soil. Biologische Bundesanstalt für Land- und Forstwirtschaft (BBA), Richtlinien für die Prüfung von Pflanzenschutzmitteln in Zulassungsverfahren, Test Guideline Part IV, 4-1, Saphir Verlag, Ribbesbüttel, Germany.

BBA (1990a). Degradability and Fate of Plant Protection Agents in the Water/Sediment System for Simulation of Smaller Surface Waters. Biologische Bundesanstalt für Land- und Forstwirtschaft (BBA), Richtlinien für die Prüfung von Pflanzenschutzmitteln in Zulassungsverfahren, Test Guideline Part IV, 5-1, Saphir Verlag, Ribbesbüttel, Germany.

BBA (1990b). Auswirkungen auf die Aktivität der Bodenmikroflora. Biologische Bundesanstalt für Land- und Forstwirtschaft (BBA), Richtlinien für die Prüfung von Pflanzenschutzmitteln in Zulassungsverfahren, Test Guideline Part VI, 1-1, Saphir Verlag, Ribbesbüttel, Germany.

BBA (1990c). Bestimmung der Reproduktionsleistung von *Folsomia candida* (Willem) in künstlichem Boden (Draft). Biologische Bundesanstalt für Land- und Forstwirtschaft (BBA), Berlin.

Belfroid A, Seinen W, van Gestel K, Hermens J and van Leeuwen K (1995). Modelling the accumulation of hydrophobic organic chemicals in earthworms. Application of the equilibrium partitioning theory. Environ. Sci. Pollut. Res. **2**, 5-15.

Biddinger GR and Gloss SP (1984). The importance of trophic transfer in the bioaccumulation of chemical contaminants in aquatic ecosystems. Residue Review **91**, 103-145.

Brandes LJ, den Hollander H, van de Meent D (1996). SimpleBox 2.0: a Nested Multimedia Fate Model for Evaluating the Environmental Fate of Chemicals. National Institute of Public Health and Environmental Protection (RIVM), RIVM Report 719101 029, Bilthoven, The Netherlands.

Bringmann G and Kühn R (1960). Vergleichende toxikologische Befunde an Wasser-Bakterien. Gesundheits-Ingenieur **11**, 337-340.

Bringmann G and Kühn R (1980). Comparison of the toxicity tresholds of water pollutants to bacteria, algae and protozoa in the cell multiplication inhibition test. Wat. Res. **14**, 231-241.

BUA (1992). OH Radicals in the Troposphere. GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance, BUA Report 100, April 1992.

Burton GA Jr (1991). Assessing the toxicity of fresh water sediments. Environ. Toxicol. Chem. 10(2), 1585-1627.

Burton GA Jr (1992). Biological Test Method: Acute Test for Sediment Toxicity using Marine or Estuarine Amphipods. Environment Canada, Report EPS 1/RM/26, Ottawa, Ontario, Canada.

Campbell PJ, Arnold DJS, Brock TCM, Grandy NJ, Heger W, Heimbach F, Maund SJ and Streloke M (1999). Guidance Document on Higher-tier Aquatic Risk Assessment for Pesticides (HARAP). SETAC-Europe Publication, Brussels.

CCME (1998). Protocol for the Derivation of Tissue Residue Guidelines for the Protection of Wildlife that Consume Aquatic Biota. Canadian Council of Ministers of the Environment (CCME), Winnipeg, Manitoba, Canada.

Ciareli S, van Straalen NM, Klap VA and van Wezel AP (1999). Effects of sediment bioturbation by the estuarine amphipod corophium volutator on fluoranthene resuspension and transfer into mussel (Mytilus edulis). Environ. Toxicol. Chem. **18**, 318-328.

Ciareli S, Kater BJ, van Straalen NM (2000). Influence of bioturbation by the amphipod corophium volutator on fluoranthene uptake in the marine polychaete nereis virens. Environ. Toxicol. Chem. **19**, 1575-1581.

Clark KE and Mackay D (1991). Dietary uptake and biomagnification of four chlorinated hydrocarbons by guppies. Environ. Toxicol. Chem. **10**, 1205-1217.

Connell DW and Markwell RD (1990). Bioaccumulation in the soil to earthworm system. Chemosphere **20**, 91-100.

Dahllöff I, Blanck H and Hall P (1999). Short-term effects of tri-n-butyl-tin on marine sediment samples using nutrient fluxes as effect indicators. Environ. Toxicol. Chem. **18**, 850-857.

Danish EPA (2001). Waste Related Emission Scenarios for Risk Assessment of Chemicals. Baun A (ed). Danish EPA, Copenhagen, Denmark, (in prep.).

De Greef J and de Nijs ACM (1990). Risk Assessment of New Chemical Substances. Dilution of effluents in the Netherlands. National Institute of Public Health and Environmental Protection (RIVM), RIVM Report 670208001, Bilthoven, The Netherlands.

De Leeuw FAAM (1993). Assessment of the atmospheric hazards and risks of new chemicals: procedures to estimate "hazard potentials". Chemosphere **27**(8), 1313-1328.

Di Toro DM, Zarba CS, Hansen DJ, Berry WJ, Schwarz RC, Cowan CE, Pavlou SP, Allen HE, Thomas NA, Paquin PR (1991). Technical basis of establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. Environ. Toxicol. Chem. **10**, 1541-1583.

EC (1996). Technical Guidance Document in support of the Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No 1488/94 on Risk Assessment for Existing Substances. Parts 1-4. Office for Official Publications of the EC, Luxembourg.

EC (1999). Study on the Prioritisation of Substances Dangerous to the Aquatic Environment: II Assessment of Options of the Statistical Treatment and Evaluation of Monitoring Data within the COMMPS Procedure. Office for Official Publications of the EC, Luxembourg.

EC (2001). Expert Consultation Workshop on Statistical Extrapolation Techniques for Environmental Effects Assessments. Report of the London Workshop, 17-18th January, 2001. European Commission, Joint Research Center, Institute for Health and Consumer Protection, European Chemicals Bureau, Ispra (VA), Italy, 9 p.

ECETOC (1993). Assessment of the Biodegradation of Chemicals in the Marine Environments. European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Technical Report No. 54, Brussels.

ECETOC (1994a). Aquatic Toxicity Data Evaluation. European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Technical Report No. 56, Brussels.

ECETOC (1994b). Environmental Exposure Assessment. European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Technical Report No. 61, Brussels.

ECETOC (2000). Comparative Ecotoxicity of Chemicals to Freshwater and Saltwater Organisms. Background paper provided to the TGD working group on Marine Risk Assessment. European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Brussels.

ECETOC (in press). The Role of Bioaccumulation in Environmental Risk Assessment: The Aquatic Environment and the Related Food Web. European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Technical Report No. 68, Brussels.

Eijsackers HJP (1989). The Netherlands Integrated Soil Research Programme: Plan and Realization of the Research Programme. Programme Office for Integrated Soil Research, Wageningen, The Netherlands.

Finizio A, Mackay D, Bidleman T and Hamer T (1997). Octanol-air partition coefficient as a predictor of partitioning of semi-volatile organic chemicals to aerosol. Atmospheric Environment **30**, 2289-2296.

Elf & IARE (1996). Biodegradability of chemical substances in seawater. Results of the OSPARCOM ring test. Prepared by Elf Akvamiljo & Institut des Aménagements Régionaux et de l'Environnement (IARE).

Emans HJB, Van De Plassche EJ, Canton JH, Okkerman PC, Sparenburg PM (1993). Validation of some extrapolation methods used for effect assessment. Environ. Toxicol. Chem. **12**, 2139-2154.

Esser HO and Mosser P (1982). An appraisal of problems related to the measurement and evaluation of bioaccumulation. Ecotox. Env. Saf. **6**, 131-148.

Evans MS, Noguchi GE and Rice CP (1991). The biomagnification of polychlorinated biphenyls, toxaphene, and DDT compounds in a Lake Michigan offshore food web. Arch. Environ. Contam. Toxicol. **20**, 87-93.

EU Annex V Testing Methods, relevant Directives and Official Journals; ECB web page <http://ecb.jrc.it/testing-methods>.

Fisk AT, Norstrom RJ, Cymbalisty CD and Muir DCG (1998). Dietary accumulation and depuration of hydrophobic organochlorines: Bioaccumulation parameters and their relationship with the octanol/water partition coefficient. Environ. Toxicol. Chem. **17**, 951-961.

Frank R and Klöppfer W (1989). A convenient model and program for the assessment of abiotic degradation of chemicals in natural waters. Ecotox. Environ. Safety **17**, 323-332.

Heijna-Merkus E and Hof M (1993). Harmonisation of Model Parameters. National Institute of Public Health and Environmental Protection (RIVM), RIVM Report 679102022, Bilthoven, The Netherlands.

HELCOM (1998). The Third Baltic Sea Pollution Load Compilation (PLC-3). Helsinki Commission (HELCOM), Baltic Marine Environment Protection Commission. Baltic Sea Environment Proceedings No. 70, Helsinki, Finland.

Herbst T and Nendza M (2000). UBA Inventory of Marine Biotest Methods for the Evaluation of Dredged Material and Sediments. Umwelt BundesAmt Research Report 298 25 753.

Hill IR, Heimbach F, Leeuwangh P and Mathiessen P (eds.) (1994). Freshwater Field Tests for Hazard Assessment of Chemicals. Lewis Publishers, London.

Hine J and Mookerjee PK (1975). The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. J. Org. Chem. **40**(3), 292-298.

Hoekstra JA, Van Ewijk PH (1993). Alternatives for the no-observed-effect level. Environ. Toxicol. Chem. **12**, 187-194.

Horowitz A, Shelton DR, Cornell CP and Tiedje JM (1982). Anaerobic degradation of aromatic compounds in sediments and digested sludge. Dev. Ind. Microbiol. **23**, 435-444.

IFEN (1997). L'environnement littoral et marin. Institut français de l'environnement (IFEN), Collection Etudes et Travaux n° 16. Décembre 1997.

IPCS (2000). Framework for the Integration of Health and Ecological Risk Assessment. World Health Organisation (WHO), International Programme on Chemical Safety (IPCS). Draft, April 2000. Geneva.

ISO (1993). Soil Quality - Effects of Pollutants on Earthworms (*Eisenia fetida*) - Part 2: Method for the Determination of Effects on Reproduction. International Organisation for Standardisation (ISO), Draft International Standard.

ISO (1989). Water Quality - Method for Assessing the Inhibition of Nitrification of Activated Sludge Microorganisms by Chemicals and Waste Waters. International Organisation for Standardisation (ISO), No. 9509.

ISO (1995). Water Quality – Evaluation of the "Ultimate" Anaerobic Biodegradability of Organic Compounds in Digested Sludge – Method by Measurement of the Biogas Production. International Organisation for Standardisation, No. 11734.

ISO/DIS (2001). Evaluation of the Aerobic Biodegradability of Organic Compounds at Low Concentrations – Part 1. International Organisation for Standardisation (ISO), Draft guideline No. 14592-1.

ISO/DIS (2001). Evaluation of the Aerobic Biodegradability of Organic Compounds at Low Concentrations – Part 2. International Organisation for Standardisation (ISO), Draft guideline No. 14592-2.

Jager T (1998). Mechanistic approach for estimating bioconcentration of organic chemicals in earthworms (Oligochaeta). Environmental Toxicology and Chemistry **17**(10), 2080-2090.

Jongbloed RH, Pijnenburg J, Mensink BJWG, Traas TIP and Luttik R (1994). A Model for Environmental Risk Assessment and Standard Setting Based on Biomagnification. Top Predators in Terrestrial Ecosystems. National Institute of Public Health and Environmental Protection (RIVM). RIVM Report 71901012, Bilthoven, The Netherlands.

Junge CE (1977). **In**: Fate of Pollutants in the Air and Water Environment. Suffet IH (ed), Wiley Interscience, New York, NY, 7-25.

Kaag NHBM (1998). The Role of Feeding in the Bioavailability of Sediment Bound Contaminants to Marine Benthic Invertebrates. Thesis Free University, Amsterdam.

Knacker T and Morgan E (1994). UBA Workshop on Terrestrial Model Ecosystems. Umwelt BundesAmt, UBA-FB 94-117.

Kooijman SALM (1987). A safety factor for LC50 values allowing for differences in sensitivity among species. Wat. Res. **21**, 269-276.

Källquist T (2000). Minutes from 2nd Expert Meeting on the Revision of OECD Test Guideline 201, Algae Growth Inhibition Test, Oslo, 29-30 Nov. 1999; Revision of OECD Test Guideline 201, Algae Growth Inhibition test, Progress Report May 2000 and Draft Proposal for an Update of OECD Test Guideline 201 (Dec. 2000).

Karman CC, Vik EA, Schobben HPM, Ojford GD and van Dokkum HP (1998). Charm III Main Report. Organisation for Applied Scientific Research (TNO), TNO Report TNO-MEP – R 96/355, Zeist, The Netherlands.

Léon CD and Van Gestel CAM (1994). Selection of a Set of Standardized Laboratory Toxicity Tests for the Hazard Assessment of Chemical Substances in Terrestrial Ecosystems. Vrije Universiteit, Department of Ecology and Ecotoxicology, Report No. D94004, Amsterdam.

Lewis R (1997). Dispersion in Estuaries and Coastal Waters. John Wiley & Sons Publishers, Chichester, UK, p. 312.

Løkke H and Van Gestel CAM (1993). Manual for SECOFASE, Development, Improvement and Standardization of Test Systems for Assessing Sublethal Effects of Chemicals on Fauna in the Soil Ecosystem. Report from a Workshop held in Silkeborg, Denmark, January 18-19, 1993, National Environmental Research Institute, 41 pp.

Løkke H. and Van Gestel CAM (eds) (1998). Handbook of Soil Invertebrate Toxicity Tests. Ecological and Environmental Toxicology Series, John Wiley & Sons Publishers, Chichester, UK.

Ma WC (1994). Methodological principles of using small mammals for ecological hazard assessment of a chemical soil pollution, with examples on cadmium and lead. **In**: Ecotoxicology of soil organisms. Donker MH, Eijsackers H, Heimbach F (eds), SETAC Special Publication Series, Lewis Publishers, Boca Raton, FL, USA.

Mackay D (1991). Multimedia Environmental Models. Lewis Publishers, Chelsea, MI, USA.

Mackay D, Paterson S, Shiu WY (1992). Generic models for evaluating the regional fate of chemicals; Chemosphere **24**(6), 695-717.

Madsen T, Rasmussen HB and L Nilsson (1995). Anaerobic biodegradation potentials in digested sludge, a freshwater swamp and a marine sediment. Chemosphere **31**, 4243-4258.

Mayer et al. (1996). Bioavailability of sedimentary contaminants subject to deposit feeder and digestion. Environ. Sci. Technol. **30**, 2641-2645.

Meylan WM and Howard PH (1991). Bond contribution method for estimating Henry's law constants. Environ. Toxicol. Chem. **10**, 1283 - 1293.

Meylan WM, Howard PH, Boethling RS and Aronson A (1999). Improved method for estimating bioconcentration/bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem **18**, 664-672.

Mikkelsen J (1995). Fate Model for Organic Chemicals in an Activated Sludge Wastewater Treatment Plant - Modification of SimpleTreat. National Environmental Research Institute, Denmark. Prepared for the Danish EPA.

Moss B (1988). Ecology of Fresh Waters. 2nd Edition, Blackwell Scientific Publications, Oxford.

Naton E (1989). Die Prüfung der Nebenwirkung von Pflanzenschutzmitteln auf *Aleochara bilineata Gyll.* (Col., Staphylinidae). Anzeiger für Schädlingskunde Pflanzenschutz Umweltschutz 62.

NEN (1988). Soil - Determination of the Influence of Chemicals on Soil Nitrification. Nederlandse Norm No. 5795, Nederlands Normalisatie-Instituut, Delft.

Nendza M, Herbst T, Kussatz C and Gies A (1997). Potential for secondary poisoning and biomagnification in marine organisms. Chemosphere **35**(9), 1875-1885.

Notenboom J and Boessenkool JJ (1992). Acute toxicity testing with the groundwater copecod Parastenocarsis germanica (Crustecea). **In**: Proceedings of the 1st International Conference on Groundwater Ecology. Stanford JA and Simons JJ (eds). American Water Resources Association, Bethesda, MD, USA, pp. 301-309.

Nyholm N (1985). Response variable in algal growth inhibition tests - Biomass or growth rate? Water Res. **19**(3), 273-279.

Nyholm N amd Källquist T (1989). Methods for growth inhibition tests with freshwater algae. Environ. Toxicol. Chem. **8**, 689-703.

OECD (1981a). Bioaccumulation: Flow-through Fish Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 305E, Paris.

OECD (1981b). Simulation test - Aerobic Sewage Treatment, Coupled Unit Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 303A, Paris.

OECD (1981c). Guidelines for Testing of Chemicals. Organisation for Economic Cooperation and Development (OECD), (including 1984 and 1987 updates), Paris.

OECD (1981d). Inherent Biodegradability (A: Modified SCAS Test, C: Zahn-Wellens/Modified MITI Test (II)). Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 302A-C, Paris.

OECD (1984a). Alga, Growth Inhibition Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 201, Paris.

OECD (1984b). Daphnia sp., Acute Immobilisation Test and Reproduction Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 202, Paris.

OECD (1984c). Fish, Prolonged Toxicity: 14-day Study. Organisation for Economic Cooperation and Development (OECD), Guideline for the Testing of Chemicals No. 204, Paris.

OECD (1984d). Earthworm Acute Toxicity Test. Organisation for Economic Cooperation and Development (OECD), Guideline for the Testing of Chemicals No. 207, Paris.

OECD (1984e). Terrestrial Plants, Growth Test. Organisation for Economic Cooperation and Development (OECD), Guideline for the Testing of Chemicals No. 208 (update proposal: July 2000), Paris.

OECD (1984f). Activated Sludge, Respiration Inhibition Test. Organisation for Economic Cooperation and Development (OECD), Guideline for the Testing of Chemicals No. 209, Paris.

OECD (1984g). Fish, Early-life Stage Toxicity Test. Organisation for Economic Cooperation and Development (OECD), Guideline for the Testing of Chemicals No. 210, Paris.

OECD (1984h). Avian Dietary Toxicity Test. Organisation for Economic Cooperation and Development (OECD), Guideline for the Testing of Chemicals No. 205, Paris.

OECD (1984i). Avian Reproduction Test. Organisation for Economic Cooperation and Development (OECD), Guideline for the Testing of Chemicals No. 206, Paris.

OECD (1989). Report of the OECD Workshop on Ecological Effects Assessment. Organisation for Economic Cooperation and Development (OECD), OECD Environment Monographs No. 26, Paris.

OECD (1992a). Screening Assessment Model System (SAMS), Version 1.1. Organisation for Economic Cooperation and Development (OECD), Paris.

OECD (1992b). Report of the OECD Workshop on Effects Assessment of Chemicals in Sediment. Organisation for Economic Cooperation and Development (OECD), OECD Environment Monographs No. 60, Paris.

OECD (1992c). The Rate of Photochemical Transformation of Gaseous Organic Compounds in Air Under Tropospheric Conditions. Organisation for Economic Cooperation and Development (OECD), OECD Environment Monographs No. 61, Paris.

OECD (1992d). Report of the OECD Workshop on the extrapolation of laboratory aquatic toxicity data on the real environment. Organisation for Economic Cooperation and Development (OECD), OECD Environment Monographs No 59, Paris.

OECD (1992e). Biodegradability in Seawater. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 306, Paris.

OECD (1992f). Ready Biodegradability. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 301A-F, Paris.

OECD (1992g). Inherent Biodegradability: Zahn-Wellens/EMPA Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 302B, Paris.

OECD (1993a). Application of Structure-Activity Relationships to the Estimation of Properties Important in Exposure Assessment. Organisation for Economic Cooperation and Development (OECD), OECD Environment Monographs No. 67, Paris.

OECD (1993b). OECD Guidelines for Testing of Chemicals. Organisation for Economic Cooperation and Development (OECD), Paris.

OECD (1996). Bioaccumulation: Flow-through Fish Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 305, Paris.

OECD (1995). Terrestrial Effects Working Group Meeting, Paris 18-19 June 1995. Draft summary of discussions. Organisation for Economic Cooperation and Development (OECD), Paris.

OECD (1998a). Detailed Review Paper on Aquatic Testing Methods for Pesticides and Industrial Chemicals. Organisation for Economic Cooperation and Development (OECD), OECD Environmental Health and Safety Publications. Series on Testing and Assessment No. 11, Paris.

OECD (1998b). *Daphnia magna* Reproduction Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 211, Paris.

OECD (1998c). Fish, Short-term Toxicity Test on Embryo and Sac-fry Stages. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 212, Paris.

OECD (2000a). Adsorption – Desorption using a Batch Equilibrium Method, updated Guideline. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 106, Paris.

OECD (2000b). Aerobic and Anaerobic Transformation in Soil, draft Guideline. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 307, Paris.

OECD (2000c). Aerobic and Anaerobic Transformation in Aquatic Sediment Systems. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 308 (draft), Paris.

OECD (2000d). Fish, Juvenile Growth Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 215, Paris.

OECD (2000e). Soil Microorganisms: Nitrogen Transformation Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 216, Paris.

OECD (2000f). Soil Microorganisms: Carbon Transformation Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 217, Paris.

OECD (2000g). Log Kow pH-metric Method for Ionisable Substances. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals, Proposal for a new Test Guideline 122 (draft November 2000), Paris.

OECD (2000h). Long-term test on Enchytraeidae. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals, Proposal for a new Test Guideline 220 (draft March 2000), Paris.

OECD (2000i). Earthworm reproduction test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals (draft January 2000), Paris.

OECD (2000j). Terrestrial (Non-Target) Plant Test: 208 A: Seedling Emergence and Seedling Growth Test; 208 B: Vegetative Vigour Test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals, Proposal for updating Guideline 208 (draft July 2000), Paris.

OECD (2000k). Report of the OECD Workshop on Improving the Use of Monitoring Data in the Exposure Assessment of Industrial Chemicals. Organisation for Economic Cooperation and Development (OECD), OECD Environmental Health and Safety Publications, Series on Testing and Assessment No. 18, Paris.

OECD (2001a). Estimation of Adsorption Coefficient (Koc) on Soil and Sewage Sludge using HPLC, original Guideline, Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 121, Paris.

OECD (2001b). Simulation test - Aerobic Sewage Treatment, Activated Sludge Units. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 303A (updated Guideline), Paris.

OECD (2001c). Guidance Document on the Use of the Harmonized System for the Classification of Chemicals which are Hazardous for the Aquatic Environment. Organisation for Economic Cooperation and Development (OECD), OECD Environmental Health and Safety Publications, Series on Testing and Assessment, No. 27.

OECD (2001d). Aerobic Mineralisation in surface water – simulation biodegradation test. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 309 (draft September 2001), Paris.

OECD (2001e). Chironomid Toxicity Test using Spiked Sediment. Organisation for Economic Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals No. 218 (draft), Paris.

Oetken M, Ludwichowski KU, Nagel R (2000). Sediment Tests with Lumbriculus Variegatus and Chironomus Riparius and 3,4-Dichloroaniline (3,4-DCA) within the Scope of EG-Altstoff-V. By order of the Federal Environmental Agency, FKZ 360 12 001, March 2000.

Opperhuizen A (1991). Bioconcentration and biomagnification: Is a distinction necessary? **In**: Bioaccumulation in aquatic systems. Nagel R and Loskill R (eds). VCH Publishers, Weinheim, Germany.

OSPAR (1998). OSPAR Strategy with Regard to Hazardous Substances. OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic, Summary Record OSPAR 98/14/1, Annex 34.

OSPAR (2000a). Decision 2000/2 on a Harmonised Mandatory Control System for the Use and Reduction of the Discharge of Offshore Chemicals, OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic.

OSPAR (2000b). Decision 2000/3 on the Use of Organic Phase Drilling Fluids and the Discharge of OPF-Contaminated Cuttings. OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic.

Pack S. (1993). A review of statistical data analysis and experimental design in OECD aquatic toxicology test guidelines. Shell Research, Sittingbourne, UK, prepared for OECD.

Pearce PA, Elliott JE, Peakall DB, Norstrom RJ (1989). Organochlorine contaminants in eggs of seabirds in the Northwest Atlantic, 1968-1984. Environmental Pollution **56**, 217-235.

Pedersen F, Kristensen P, Damborg A and Christensen HW (1994). Ecotoxicological Evaluation of Industrial Wastewater. Ministry of the Environment, Danish Environmental Protection Agency, Miljøprojekt Nr. 254, pp. 80-81.

Posthuma L, Suter GW and Traas TP (2001). Species Sensitivity Distributions in Ecotoxicology. CRC Press, Boca Raton, FL, USA.

Rasmussen JB, Rowan DJ, Lean DRS and Carey JH (1990). Food chain structure in Ontario lakes determine PCB levels in lake trout (*Salvelinus namaycush*) and other pelagic fish. Canadian Journal of Fisheries and Aquaculture Science **47**, 2030-2038.

Ratte HT (1998). Influence of the Growth Pattern on the EC50 of Cell Number, Biomass Integral and Growth rates in the Algal Growth Inhibition Test, Vol. I (Anonymised version). UBA Project 360 030 10, Aachen, Germany, October 1998.

Reynolds L, Blok J, de Morsier A, Gerike P, Wellens H and Bonontinck WJ (1987). Evaluation of the toxicity of substances to be assessed for biodegradability. Chemosphere **16**, 2259-2277.

Römbke J, Bauer C, Brodesser J, Brodsky J, Danneberg G, Dietze C, Härle M, Heimann D, Klunker H, Kohl EG, Renner I, Ruzicka J, Schallnass HJ, Schäfer H, Vickus P (1993). Grundlagen für die Beurteilung des ökologischen Gefährdungspotentials von Altstoffen im Medium Boden, Entwicklung einer Teststrategie, Bericht im Auftrag des Umweltbundesamtes, F + E - Vorhaben Nr. 106 04 103, Batelle Europe, Frankfurt am Main.

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.

Romijn CFAM, Luttik R, Canton JH (1994). Presentation of a general algorithm to include effect assessment on secondary poisoning in the derivation of environmental quality criteria. Part 2. Terrestrial food chains. Ecotox. Environ. Saf. **27**, 107-127.

Rundgren S, Andersson R, Bringmark L, Byman J, Gustafsson K, Johansson I and Tortensson L (1989). Soil Biological Variables in Environmental Hazard Assessment: Organisation and Research Programme. National Swedish Environmental Protection Board, NSEPD Report No. 3603, Solna, Sweden.

Russell FS and Yonge CM (1928). The Seas. Frederick Warne and Co. Ltd, London.

Samsøe-Petersen L (1987). Laboratory method for Ttesting side-effects of pesticides on the rove beetle *Aleochara bilineata* - adults (Col., Staphylinidae). Entomophaga **32**, 73-81.

Samsøe-Petersen L, Pedersen F (1994). Discussion paper regarding Guidance for Terrestrial Effects Assessment. VKI, prepared for the Organisation for Economic Cooperation and Development (OECD). 63 pp.

SCB (2000). Vattenräkenspaper – en pilotstudie om uttag, användning samt utsläpp, fysika och monetära data. Statistiska centralbyrån (SCB), Rapport 2000: 6. Stockholm, (Water accounts – a pilot study on physical and monetary data on withdrawal, use and emissions. Stockholm, Statistics Sweden. Report in Swedish).

Schobben HPM, Karman CC and Scholten MCTh (1994). Charm 2.1: Chemical Hazard Assessment and Risk Managment of Offshore Exploration and Production Chemicals. Organisation for Applied Scientific Research (TNO), TNO Report TNO-MW-R94/315, Delft, The Netherlands.

Schudoma D, Gies A, Kussatz C (1999). Ableitung von Qualitätskriterien zum Schutz von fisch- und muschelfressenden Tierarten. **In**: Ökotoxikologie: ökosystemare Ansätze und Methoden. Oehlamnn J, Markert B (eds). Ecomed Verlag, Landsberg.

Schwarzenbach RP, Gschwend PM and Imboden DM (1993). Environmental Organic Chemistry. Wiley-Interscience, New York, NY.

SETAC (1991). Guidance Document on Testing procedures for Pesticides in Freshwater Mesocosms. Society of Environmental Toxicology and Chemistry (SETAC), (Publication available at http://www.setac.org).

SETAC (1992). Workshop on Aquatic Microcosms for Ecological Assessment of Pesticides, Wintergreen, Virginia, 6 - 12 October 1991. Society of Environmental Toxicology and Chemistry (SETAC), Workshop Report.

SETAC (1993). Guidance Document on Sediment Toxicity Tests and Bioassays for Freshwater and Marine Environments. From the Workshop on Sediment Toxicity Assessment at Renesse, Netherlands on 8-10 November 1993. Hill I, Mathiessen P, Heimbach F (eds). Society of Envionmental Toxicology and Chemistry – Europe, Brussels.

SETAC (1995). Guidance Document on Regulatory Testing Procedures for Pesticides with non-target Arthropods. Stavola A (1990). Detailed Review Paper on Terrestrial Ecotoxicology Test Guidelines. OECD Updating Programme, periodical review.

SRC (2000). EPIWIN Suite 3.05. Syracuse Research Corporation (http://esc.syrres.com/interkow/Softwareupdate.htm).

Stavola A (1990). Detailed Review Paper on Terrestrial Ecotoxicology Test Guidelines, OECD Updating Programme, periodical review.

Stronkhorst J, Ciarelli S, Schipper CA, Postma JF, Dubbeldam M, Vangheluwe M, Brils JM, Hooftman R and Kater BJ (in press). Interlaboratory comparison of five marine bioassays for the toxicity evaluation of dredged material in the Netherlands.

Struijs J, Stoltenkamp J, Van De Meent D (1991). A Spreadsheet-based Model to Predict the Fate of Xenobiotics in a Municipal Wastewater Treatment Plant. Wat. Res. **25**(7), 91-900.

Tait RV (1978). Elements of Marine Ecology. Butterworths, London.

Teigen WS, Skaare JU, Bjorge A, Degre E and Sand G (1993). Mercury and selenium in harbor porpoise (*Phocoena phocoena*) in Norwegian waters. Environ. Toxicol.Chem. **12**, 1251-1259.

Thain J and Bifield S (2001). Biological effects of contaminants: A Sediment Bioassay using the Polychaete Arenicola marina. International Council for the Exploration of the Sea (ICES), ICES Techniques in Marine Environmental Sciences No. 29, Copenhagen, 16 pp.

Thompson DR (1990). Metal levels in marine vertebrates. **In**: Heavy Metals in the Marine Environment. Furness RW and Rainbow PS (eds). CRC Press, Boca Raton, FL, USA.

TNsG on Annex I Inclusion (2001). Technical Notes for Guidance in Support of the Directive 98/8/EC of the European Parliament and the Council Concerning the Placing of Biocidal Products on the Market. Principles and Practical Procedures for the Inclusion of Active Substances in Annexes I, IA and IB. European Commission (EC) (Internet publication at http://ecb.jrc.it).

TNsG on Data Requirements (2000). Technical Guidance Document in Support of the Directive 98/8/EC Concerning the Placing of Biocidal Products on the Market. Guidance on Data Requirements for Active Substances and Biocidal Products. European Commission (EC) (Internet publication at http://ecb.jrc.it).

Toet C, de Nijs ACM, Vermeire TG, van der Poel P and Tuinstra J (1991). Risk Assessment of New Chemical Substances; System Realisation and Validation II. National Institute of Public Health and the Environment (RIVM), RIVM Report No. 679201 004, Bilthoven, The Netherlands.

Toet C and de Leeuw FAAM (1992). Risk Assessment System for New Chemical Substances: Implementation of atmospheric transport of organic compounds. National Institute of Public Health and Environmental Protection (RIVM), RIVM Report No. 679102 008, Bilthoven, The Netherlands.

UBA (1993). Entwurf zur Bewertung von Bodenbelastungen, Fachgebiet I 3.7. Umweltbundesamt (UBA), Berlin.

US EPA (1973). Biological Field and Laboratory Methods for Measuring the Quality of Surface Waters and Effluents. US Environmental Protection Agency (US EPA), Office and Research and Development, EPA 670/4-73-001, Cincinnati, OH, USA.

US EPA (1978). Bioassay Procedures for the Ocean Disposal Permit Program. US Environmental Protection Agency (US EPA), Office and Research and Development, EPA 600/9-78-010, Cincinnati, OH, USA.

US EPA (1980). Chemical Use Standard Encoding System (ChemUSES), Volume 2: Function List and Function List Index. US Environmental Protection Agency (US EPA), Office of Toxic Substances, Doc. EPA 560/13-80-034b, Washington, DC.

US EPA (1985). Water quality criteria. US Environmental Protection Agency (US EPA), Fed. Regist. 50, 30784-30796.

US EPA (1996). Whole Sediment Acute Toxicity Invertebrates, Marine. US Environmental Protection Agency (US EPA), Office of Prevention, Pesticides and Toxic Substances (OPPTS), Ecological Effects Test Guidelines OPPTS 850.1740, EPA 712-C-96-355, Washington, DC.

US EPA (2002). US Environmental Protection Agency (US EPA). Available from the US EPA website: http://www.epa.gov/oppt/exposure/docs/episuitedl.htm.

Van Beelen P, Fleuren-Kemilä AK, Huys MPA, Van Mil ACM and Van Vlaardingen PLA (1990). Toxic effects of pollutants on the mineralization of substrates at low experimental concentrations in soil, subsoils and sediments. **In**: Contaminated Soil. Arendt F, Hinseveld M and Van den Brink WJ (eds). Kluwer Academic Publishers, The Netherlands, pp. 431-438.

Van de Meent D and Toet C (eds.) (1992). Dutch Priority Setting System for Existing Chemicals: a Systematic Approach for Ranking Chemicals according to Increasing Estimated Hazards. National Institute of Public Health and the Environment (RIVM), RIVM Report No. 679120 001, Bilthoven, The Netherlands.

Van de Meent D (1993). Simplebox: a Generic Multimedia Fate Evaluation Model. National Institute of Public Health and the Environment (RIVM), RIVM Report No. 672720 001, Bilthoven, The Netherlands.

Van der Poel P (1999). Supplement to the Uniform System for the Evaluation of Substances (USES) - Emission Scenarios for Waste Treatment (elaborated for biocides). National Institute of Public Health and the Environment (RIVM), RIVM Report No. 601450 003, Bilthoven, The Netherlands.

Van Gestel CAM (1992). The influence of soil characteristics on the toxicity of chemicals for earthworms: a review. **In**: Ecotoxicology of Earthworms. Becker H et al. (eds), Intercept, Andover, UK, pp. 44-54.

Van Gestel CAM, and Ma W (1993). Development of QSARs in soil ecotoxicology: earthworm toxicity and soil sorption of chlorophenols, chlorobenzenes and chloroanilines. Water, Air and Soil Pollution **69**, 265-276.

Van Jaarsveld JA (1990). An operational atmospheric transport model for Priority Substances; specifications and instructions for use. National Institute of Public Health and the Environment (RIVM), RIVM Report No. 222501002, Bilthoven, The Netherlands.

Van Straalen NM and Denneman CAJ (1989). Ecotoxicological evaluation of soil quality criteria. Ecotoxicol. & Environ. Saf. **18**, 241-251.

Van Straalen NM and Van Gestel CAM (1992). Ecotoxicological Test Methods Using Terrestrial Arthropods. Detailed Review Paper for the OECD Test Guidelines Programme, Amsterdam.

Veith GD, Defoe DL and Bergstedt BV (1979). Measuring and estimating the bioconcentration factor of chemicals in fish. J. Fish Board Can. **36**, 1040-1048.

Vermeire TG, van Iersel AAJ, de Leeuw FAAM, Peijnenburg WJGM, van der Poel P, Taalman RDFM and Toet C (1992). Initial assessment of the hazards and risks of new chemicals to man and the environment. National Institute of Public Health and the Environment (RIVM), RIVM Report No. 679201 006, Bilthoven, The Netherlands.

Voparil IM and Mayer LM (2000). Dissolution of sedimentary polycyclic aromatic hydrocarbons into the lugworm's (*Arenicola marina*) digestive fluids. Environ. Sci. Technol. **34**(7), 1221-1228.

Wagner C and Løkke H (1991). Estimation of ecotoxicological protection levels from NOEC toxicity data. Water Res. **25**, 1237-1242.

Weyers A and Vollmer G. (2000). Algal growth inhibition: Effect of choice of growth rate for biomass as endpoint on the classification and labelling of new substances notified in the EU. Chemosphere **41**, 109-112.

Weyers A, Sokull-Klüttgen B, Baraibar-Fentanes J and Vollmer G (2000). Acute toxicity data: A comprehensive comparison of results of fish, Daphnia and algae tests with new substances notified in the EU. Environmental Toxicology and Chemistry **19**, 1931-33.

Xie WH, Shiu WY and Mackay D (1997). A review of the effects of salts on the solubility of organic compounds in seawater. Marine Env. Res. **44**, 429-444.

Zepp GR and Cline DM (1977). Rates of direct photolysis in aquatic environment. Environ. Sci. Techn. **11**(4), 359-366.

Appendix 1 - 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 Spp.*, *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 constituents.

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 reasons 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 2 - 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 2-1: 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 3 - 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.

Table 3-1:

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 4 - Connection to Sewage 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) followed full implementation of the Urban Waste Water Treatment Directive (91/271/EEC) in 2005. The proportion of the population connected to urban wastewater treatment covers those households that are connected to any kind of sewage treatment. This share was above 80 % in approximately half of the EU Member States for which data are available (mixed reference years), rising to 99 % in the Netherlands, 97 % in England and Wales, and 95 % in Germany and Luxembourg, while Switzerland (97 %) also recorded a high connection rate. At the other end of the range, less than one in two households were connected to urban wastewater treatment in Malta, Bulgaria, Cyprus and Romania as well as in Croatia and the former Yugoslav Republic of Macedonia; new treatment plants are under construction in Malta and it is expected that this will result in high connection rates soon (Eurostat, 2012).

Based on these data, a figure of 90% connection to wastewater treatment is therefore proposed for the generic region. A figure of 90 - 95% was also proposed in the TGD (2003) 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.

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 4-1. 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 % in Greece, 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)

Table 4-1: 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

In terms of treatment levels tertiary wastewater treatment was most common (again mixed reference periods) in the Netherlands, Germany, Austria, Sweden and Greece, where at least four in every five persons were connected to this type of wastewater treatment. By contrast, no more than 1 % of the population was connected to tertiary wastewater treatment in Bulgaria.

The residual of wastewater treatment is sewage sludge. While the amount of sludge generated per inhabitant depends on many factors and hence is quite variable across countries, the nature of this sludge – rich in nutrients, but also often loaded with high concentrations of pollutants such as heavy metals – has led countries to seek different pathways for its disposal. Typically, four different types of disposal make up a considerable share of the total volume of sewage sludge treated: more than two thirds of the total was used as fertiliser in agriculture in Spain and Ireland, while another eight Member States (Lithuania, Hungary, Bulgaria, Cyprus, Luxembourg, France, the Czech Republic and Latvia), as well as Norway, reported between one and two thirds of their total mass of sewage sludge being disposed of through agricultural uses. By contrast, more than two thirds of sewage sludge was composted in Estonia and Slovakia. Otherwise, alternative forms of disposal may be used to reduce or eliminate the spread of pollutants on agricultural or gardening land; these include incineration and landfill. While the Netherlands, Slovenia, Belgium, Germany and Austria (as well as Switzerland) reported incineration as their primary pathway for disposal, its discharge into controlled landfills was practised as the primary pathway in Greece, and was used exclusively in Malta (Eurostat, 2012).

Appendix 5 - Information on the difference in diversity between seawater and freshwater

The greater diversity of species in seawaters[16] 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 seawater 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 seawater)
Cnidaria	7,000	(Exclusively seawater)
Tubellaria	2000	(1000 in freshwater)
Trematoda	6,000 (internal parasites)	------
Cestoda	3,500 (internal parasites)	------
Nemateans	900	(Predominantly seawater)
Gastrotricha	150	(sea and fresh water)
Nematoda	5,000	(15,000 described species in total including parasites and terrestrial, sea- and freshwater forms)
Nematomorpha	4	(316 in freshwater)
Achantocephala	1,150 (internal parasites)	-----
Kinorhyncha	150	(Exclusively seawater)
Priapulida	17	(Exclusively seawater)
Loricifera	100	(Exclusively seawater)
Gnatostomolida	80	(Exclusively seawater)
Rotifera	100	(1,400 in freshwater)
Polychata	5-10,000	(1000 in freshwater)
Oligochaeta	------	(Many species; mainly in freshwater)
Echinodermata	7,000	(Exclusively seawater)
Brachiopoda	300	(Exclusively seawater)
Echiura	140	(Exclusively seawater)
Sipunculida	350	(Exclusively seawater)
Pogonophora	120	(Exclusively seawater)
Tardigrada		(Taxonomic group discovered a few decades ago. A few hundred species

16 Except those where there are extremes of environmental conditions

Taxonomic group	No. of species	Comments
		known from both terrestrial, fresh- and seawater)
Arthropoda		
Chelicerata		
Merostomata	4	(Exclusively seawater)
Pygnogonida	1,000	(Exclusively seawater)
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 seawater)
Cephalopoda	600	(Exclusively seawater)
Bryozoa	5,000	(70 in freshwater)
Hemichordata	100	(Exclusively seawater)
Chordata		
Tunicata	1,300	(Exclusively seawater)
Cephalocordata	25	(Exclusively seawater)
Vertebrata		
Pisces	15,000	(Guestimate but believed to be an underestimate number of freshwater species less than number of seawater species)
Amphibians		(Mainly freshwater)
Mammals	60	(Guestimate)

Appendix 6 - $PNEC_{oral}$ derivation for the primary and secondary poisoning assessment of anti-coagulant rodenticides

Derivation of $PNEC_{oral}$ for primary and secondary poisoning has been discussed at the Biocides Technical Meeting I in 2006 when discussing the substances difethialone and coumatetralyl. Norway provided a discussion document which resulted in the following guidance.

There was a general agreement that the principles laid down in the TGD do not reflect the special situation with regard to rodenticides very well. In addition to the secondary poisoning assessment from the TGD (PEC_{oral}, fish and PEC_{oral}, worm compared to a PNEC for fish- or worm-eating mammals or birds) another food chain rodenticide (bait) or rodent or rodent-eating mammal or rodent-eating bird has to be assessed here. A predicted environmental concentration, which corresponds to the PEC_{oral}, predator in the TGD needs to be defined. According to the emission scenario developed for product-type 14 in the EUBEES project "…it will then be compared with the predicted no-effect concentration $PNEC_{oral}$ according to the TGD". However, the guidance for PNEC derivation given in the TGD refers to an exposure situation which is completely different from the exposure situation for rodenticides. Also in the ESD PT14 it is questioned "…if the $PNEC_{oral}$ calculated according to the TGD is really very suitable for rodenticides".

One issue not yet discussed at TM regarding $PNEC_{oral}$ derivation for the primary and secondary poisoning assessment of rodenticides is whether it is considered necessary to derive separate $PNEC_{oral}$ for an acute and a chronic exposure situation to rodenticides as done by most MS.

In ESD PT14 it is stated that "…it could be argued that both an acute and a chronic risk assessment should be done for anticoagulants, because although the mode of action is generally chronic, some anticoagulants have substantial acute toxicity." ESD PT14 states also that "…the time periods implied by the exposure and effects assessments should be comparable. If possible these two should be made consistent". The ESD PT14 gives no clear guidance on whether two separate $PNEC_{oral}$ values have to be derived and on how to do this.

The $PNEC_{oral}$ derivation described in the TGD for the secondary poisoning assessment considers the oral intake of a chemical via fish or worms and a more or less continuous exposure situation and no guidance is given at all regarding primary poisoning. The TGD does not state to derive a separate short-term $PNEC_{oral}$ in addition to the long-term $PNEC_{oral}$. Therefore no guidance is available on how to derive a short-term $PNEC_{oral}$.

At TM I '06 it was not possible to find another way of deriving $PNEC_{oral}$ than the approach described in the TGD and it was agreed to follow the TGD. However, for the short-term exposure and for primary poisoning no guidance is given in the TGD.

This Appendix provides a proposal for harmonising the primary and secondary poisoning assessment of anticoagulant rodenticides so that a future comparative assessment of anticoagulant rodenticides would be possible. .

Item 1: Do we need both a short-term and a long-term $PNEC_{oral}$?

As described in general in the TGD only one PNEC is derived for any effects assessment, which, if not exceeded, should ensure an overall protection of the environment. This PNEC can be considered as a long-term value.

The situation with respect to anticoagulant rodenticides is different. Most anticoagulant rodenticides are acutely toxic to mammals and birds and there is the possibility of an acute poisoning situation in addition to a long-term exposure of non-target mammals and birds. This situation is not reflected in the TGD, however, it is considered especially relevant for primary poisoning, whereas for secondary poisoning the long-term exposure seems to be more relevant than the acute exposure situation.

Comparing an acute poisoning incident, which represents a single uptake of the anticoagulant rodenticide by a non-target mammal or a bird, with a $PNEC_{oral}$ which has been derived in accordance with the TGD, considerably overestimates the risk due to the choice of long-term studies as a basis for deriving the $PNEC_{oral}$.

On the other hand no guidance is available on how to derive $PNEC_{oral}$ values for an acute poisoning situation. Every MS which derived short-term $PNEC_{oral}$ values for their evaluations chose its own approach. Different studies, different endpoints and different assessment factors have been used as no harmonised guidance is available at the moment. When discussing this issue it became clear that the situation is that complex that it will not be possible to reflect the real life situation in the primary and secondary poisoning assessments of the evaluation reports. It remains unclear which studies should be chosen for a derivation of an acute $PNEC_{oral}$ and also which assessment factors should be applied to them. Due to these problems it is considered more than difficult to reach a compromise regarding the derivation of a $PNEC_{oral}$ for acute poisoning situations. Having in mind the importance of harmonising the primary and secondary poisoning assessment of anticoagulant rodenticides for a future comparative assessment the following pragmatic approach is suggested for the time being. When revising the ESD PT14, guidance should be included on how to derive a $PNEC_{oral}$ for acute exposure situations.

Qualitative risk assessment for acute situation

At the moment it is suggested not to conduct a quantitative risk assessment for the acute primary as well as the acute secondary poisoning situation. Instead a qualitative description of the toxicity of the substance compared to the possible single uptake should be given.

Example primary poisoning Tier 2, single uptake without excretion:

> Concentration of a.s. in bait 25 mg/kg
>
> Tree sparrow: daily food uptake 7.6 g/day
>
> Body weight: 22 g
>
> Expected content of the a.s. in the sparrow for a single uptake incident if the sparrow consumes 100% of its daily food uptake on rodenticide bait: 8.64 mg/kg bw
>
> LD_{50} of the a.s. (bird) = 0.264 mg/kg bw

From this calculation it becomes clear that the sparrow dies if consuming 100% of its daily food uptake on rodenticide bait, even without applying an assessment factor to a single dose LD_{50}. The same comparison can be made for an acute situation at Tier 1 secondary poisoning with Frodent = 1.

It is important to stress that this qualitative assessment is not intended to be used for the risk assessment of primary and secondary poisoning of rodenticides. This comparison only gives a first indication of the acute toxicity of the substance. If an anticoagulant rodenticide with a lower acute toxicity e.g. has a LD_{50} (bird) which is above the expected content in the sparrow the conclusion of this comparison should not be that the substance is not acutely toxic or "unproblematic" with regard to the acute primary poisoning situation because a comparison is made with a single dose LD_{50} without applying an assessment factor. This comparison is not intended to be used for risk characterisation: no PNEC must be derived and hence no PEC/PNEC ratio can be established, and must not be used for a comparative assessment.

The object of a qualitative risk assessment should be:

- Primary poisoning:
    - Tier 2 for 1 days exposure with and without excretion, where the PEC_{oral} is the expected concentration of the a.s. in the non-target animal after 1 day exposure (single meal) [mg/kg bw]. A default excretion factor of 0.3 (for birds and mammals) should be used in case no data is available. For a first

step worst case, the parameter AV*, PT and PD are all 1. For a more realistic worst case AV* = 0.9, PT = 0.8 and PD = 1.

- Secondary poisoning
    - Tier 1, where the PEC_{oral} is the concentration in the rodent immediately after a last meal on day 5 [mg/kg food]. For a short-term exposure PD is 1 (rodents have fed entirely on rodenticide) and F_{rodent} = 1 (non-target animals consume 100 % of their daily intake on poisoned rodents). For comparison calculations with PD = 0.5 and PD = 0.2 could also be included.

Quantitative risk assessment for long-term situation

For the long-term exposure, as described in the ESD PT14, a quantitative risk assessment for primary and secondary poisoning should be carried out. For that the $PNEC_{oral}$ should be derived in accordance with the TGD.

The object of a quantitative risk assessment should be:

- Primary poisoning:
    - Tier 1 where the PEC_{oral} is the concentration of the actives substance in the food (bait) [mg/kg food]
    - Tier 2 for 5 days exposure, considering excretion, where the PEC_{oral} is the expected concentration of the active substance in the non-target animal after 5 days exposure [mg/kg bw]. A default excretion factor of 0.3 (for birds and mammals) should be used in case no data are available. As a worst case, the parameter AV*, PT and PD are all 1.
- Secondary poisoning
    - Tier 1 for a long-term exposure. The PEC_{oral} is the concentration in the rodent immediately after a last meal on day 5 [mg/kg food]; PD = 1 and F_{rodent} = 0.5 (non-target animals consume 50 % of their daily intake on poisoned rodents). For comparison calculations with PD = 0.5 and PD = 0.2 could also be included.
    - Tier 2 for a long-term exposure. The PEC_{oral} is the concentration in non-target animals after a single day of exposure [mg/kg bw]; PD = 1 and F_{rodent} = 0.5.

For a comparative assessment the long-term PEC/PNEC values of the respective substances should be compared. As a worst case, PEC/PNEC ratios of the smallest bird and the smallest mammal should be compared for primary as well as secondary poisoning.

Item 2: Choice of studies for the long-term risk assessment for primary and secondary poisoning

It is suggested using the NOEC from an avian reproduction study or, if not available, the LC_{50} from a 5 days feeding study with birds for $PNEC_{oral,\ bird}$ derivation.

For mammals the NOAEL from a 28 or a 90 days repeated dose toxicity study or from a chronic study should be used.

For converting the $PNEC_{oral}$ values from a concentration in food [mg/kg food] to a dose related $PNEC_{oral}$ [mg/kg body weight], and vice versa, the following equation should be used:

* AV has to be set to 0.5 for birds if the product is a paste in an envelope

Daily dose [mg/kg bw day] = conc. in food [mg/kg] · daily food consumption [g/bird day]/body weight [g]

Data from animals used in the test should be used for conversion (i.e. body weight and daily food intake of the test species) and not default values given in EUBEES.

Item 3: Assessment factors

The AF laid down in Section 3 of this Guidance should be used for $PNEC_{oral}$ derivation for the long-term risk assessment.

Appendix 7 - Tonnage based approach - Emission factors for different use categories (A&B tables of TGD, 2003)

Appendix 7 represents the former Appendix I of the TGD (2003). The TGD was prepared for chemicals and biocides. The descriptions below therefore include also the description of uses of chemicals with regard to live cycle, use classes and industrial categories. However, the emission factors also apply to biocides when the exposure assessment is performed using the tonnage based approach.

1. Introduction to the release tables

For all industrial categories estimates have been generated for:

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 have been implemented

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 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..

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 or use category documents). These emission scenario documents are presented in Chapter 7 of the TGD (2003). 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 provided in Chapter 7 of the TGD (2003)).. 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).

A substance can have applications in more than one IC and/or 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.

3. Aspects of production

If specific data on emissions at production are known, these can be used instead of the tables. 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.

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. 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.

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. 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. 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. 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 of TGD (2003) allows for one entry of the MC only, for all stages of the life-cycle.

In the context of environmental risk assessment MCs 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

(EC/OECD Harmonised Electronic Data Set) 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 7-1 interpretation is often different.

Table 7-1: 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)

Note to Table 7-1

1) Processing refers to industrial / professional use

10. Remarks on the industrial categories

This paragraph defines the scope of the 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. The cause can be divided into 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, or
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.

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 7-2: 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 7-1)

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 7-3: 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 7-1)

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 7-4: 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 7-1)

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 7-4: 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 7-1)

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 could 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 7-5: 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 7-1)

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 could 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 could 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 7-6: 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 7-1)

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 7-7: 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 7-1)

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 7-8: 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 7-1)

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 7-9: 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 7-1)

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 7-10: 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 7-1)

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 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 7-11: 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 7-1)

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 7-12: 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 7-1)

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 7-13: 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 7-1)

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 7-14: 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 7-1)

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 7-15: 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 7-1)

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 7-16: 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 7-1)

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. 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	$F_{1,a} \cdot PRODVOL$
		water	$F_{1,w} \cdot PRODVOL$
		soil	$F_{1,s} \cdot PRODVOL$
		total	$\Sigma F_{1,j} \cdot PRODVOL$
	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		Emission factors			
	Sol. (mg/l)	Vap. (Pa)	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		Emission factors			
	Sol. (mg/l)	Vap. (Pa)	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 application)	(external	0	0	0.1
41	pharmaceuticals application)	(internal	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		Emission factors			
	Sol. (mg/l)	Vap. (Pa)	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		Emission factors			
	Sol. (mg/l)	Vap. (Pa)	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	Emission factors	
	Vap. (Pa)	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 then Table A1.1 applies)

Compartment	Conditions		Emission factors	
	Sol. (mg/l)	Vap. (Pa)	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		Emission factors			
	Sol. (mg/l)	Vap. (Pa)	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			Emission factors
	Use category	Sol. (mg/l)	Vap. (Pa)	
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

Compartment	Conditions			Emission factors
	Use category	Sol. (mg/l)	Vap. (Pa)	
Air (cont.)	48, 55	<10	<10	0.005
			10-100	0.015
			100-1,000	0.15
			1,000-10,000	0.4
			≥10,000	0.6
	48, 55	10-100	<10	0.0015
			10-100	0.075
			100-1,000	0.125
			1,000-10,000	0.25
			≥10,000	0.4
	48, 55	100-1,000	<10	0.0015
			10-100	0.025
			100-1,000	0.1
			1,000-10,000	0.15
			≥10,000	0.225
	48, 55	≥1,000	<10	0.00075
			10-100	0.03
			100-1,000	0.075
			1,000-10,000	0.125
			≥10,000	0.175
Surface water	5, 35 (car products)			0.0005
Wastewater	2	25		0
		≥25		0.005
	3, 5, 19, 35			0
	7			0.01
	8 (household products)			0.95
	(cosmetics)			0.8
	9, 15			1
	50			0.99
	10 (cleaning products)			1
	(cosmetics)			0.8
	(else)			0.5
	11			0.8
	26			0.025
	36 (cosmetics)		<2,500	0.8
			2,500-10,000	0.5
			≥10,000	0.1
	(cleaning products,…)		<100	0.9
			100-2,500	0.8
			2,500-10,000	0.5
			≥10,000	0.1
	(else)		<100	0.5
			100-2,500	0.3
			2,500-10,000	0.2
			≥10,000	0.05

Table A4.1 continued

Compartment	Conditions			Emission factors
	Use category	Sol. (mg/l)	Vap. (Pa)	
Wastewater (cont.)	38 (herbicides)			0
	(pesticides, garden)			0
	(pesticides, pets)			0.1
	41 (external)			0.25
	(oral)			0.05
	47			0.9
	48, 55		<10	0.1
			10-100	0.2
			100-1,000	0.4
			≥1,000	0.6
Soil	2			0.0001
	3, 36, 41			0
	5			0.0005
	7			0.001
	8 (household products)			0.01
	(cosmetics)			0.001
	9, 15			0
	47,50			0.01
	10 (cleaning products)			0.002
	(cosmetics)			0.0001
	(else)			0.01
	11			0.0001
	19			1
	26, 35			0.002
	38 (garden: herbicides, pesticides)			0.9
	(pesticides, pets)		<100	0.05
			100-5,000	0.01
			≥5,000	0.002
	48, 55		<10	0.2
			10-100	0.1
			100-1,000	0.05
			1,000-10,000	0.005
			≥10,000	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		Emission factors		
Use categories		**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	0.015
	2,000-10,000	0.02
	10,000-100,000	0.03
	100,000-500,000	0.05
	≥500,000	0.06
Soil		0.0001

FORMULATION **Table A2.1**

INDUSTRIAL USE **Table A3.6**

Compartment	Conditions		Emission factors		
	Sol. (mg/l)	Vap. (Pa)	All MC's	MC = 2	MC = 3 1)
Air	<100	<100	0.001		
	<100	≥100	0.01		
	≥100		0		
Wastewater	<100			0.05	0.9
	100-1,000			0.15	0.99
	≥1,000			0.25	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	Emission factors
	Vap. (Pa)	
Air	<1	0.00005
	1-10	0.00001
	10-100	0.0005
	100-1,000	0.0025
	≥1,000	0.025
Wastewater		0.002
Soil		0.00001

INDUSTRIAL USE **Table A3.7**

Compartment	Conditions UC≠29&35	Emission factors	
	Sol. (mg/l)	MC = 2	MC = 3 1)
Air		0	0.25
Wastewater	<100	0.05	0.5
	100-1,000	0.1	0.5
	≥1,000	0.25	0.5
Soil		0	0.05

Compartment	Conditions UC=29&35 log Henry	Emission factors
Air	<2	0.0002
	≥2	0.002
Wastewater	Pure oils	0.185
	Water based + unknown	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	Emission factors
	Vap. (Pa)	
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	Emission factors
	Vap. (Pa)	
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	Emission factors
	Vap. (Pa)	
Air	<1	0.0001
	1-10	0.001
	10-100	0.3
	100-1,000	0.7
	≥1,000	1
Wastewater	Control of crystal growth	0.99
	Other functions	0.002
Soil		0.00025

INDUSTRIAL USE Table A3.9

Compartment	Conditions		Emission factors	
		Vap. (Pa)	MC=2	MC=3 1)
Air	Solid materials (e.g. films)		0	
	Else	<1		0.000035
		1-10		0.00025
		10-100		0.0075
		100-1,000		0.025
		≥1,000		0.075
Wastewater	Solid materials (e.g. films)		0	
	Aqueous solutions:			
	- coupler of dye			0.15
	- else			0.8
Soil	Solid materials (e.g. films)		0	
	Else			0.00025

1) Default

PRIVATE USE Table A4.3

Compartment	Conditions	Emission factors
	UC=42 (photochemicals) for aqueous solutions only	
Air		0
Wastewater		0.4
Soil		0

WASTE TREATMENT Table A5.1

Compartment	Conditions	Emission factors
	UC=42 (photochemicals) **for aqueous solutions only** **Vap. (Pa)**	
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		Emission factors		Type of
	Vap. (Pa)	Boiling point (°C)	A	B	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		Emission factors	
	Use categories	Vap. (Pa)	MC = 2	MC = 3 1)
Air	Default	<100	0	0.01
		100-1,000	0.05	0.2
		1,000-10,000	0.25	0.5
		≥10,000	0.5	0.75
	10 & 45		0	
	48	<100		0.05
		100-1,000		0.3
		1,000-10,000		0.65
		≥10,000		0.85
		Sol. (mg/l)	MC = 2	MC = 3 1)
Wastewater	Default	<100	0.0001	0.01
		100-1,000	0.005	0.05
		≥1,000	0.001	0.1
	9			0.9
	10 & 45		0.0005	
	48	<100		0.0005
		100-1,000		0.001
		≥1,000		0.005
		Vap. (Pa)	MC = 2	MC = 3 1)
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

INDUSTRIAL USE Table A3.12 for pulp, paper and board production

Compartment	Conditions			Emission factors	
	Use category	Sol. (mg/l)	Vap. (Pa)	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		Emission factors	
	Sol. (mg/l)	Vap. (Pa)	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	(UC = 10)				
Type of dye	**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		Emission factors	
	Sol. (mg/l)	Vap. (Pa)	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		Emission factors	
	Use category	Vap. (Pa)	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		Emission factors	
	Use category	Vap. (Pa)	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		Emission factors		
	Sol. (mg/l)	Vap. (Pa)	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		Field of application	
		f main source:	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·T
100-500	0.8	f·T
500-1,000	0.6	0.5f·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 ≥7,000)

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 II-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
11	Complexing agents	177	Antiprecipitants
		124	Complexing agents
		10	Sequestering agents

No.	Use Category	No.	Function (ChemUSES)
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
26	Food/feedstuff additives	214	Acidulants
		66	Feed additives
		80	Sweeteners (taste)
27	Fuels	247	Fuels

No.	Use Category	No.	Function (ChemUSES)
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
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

No.	Use Category	No.	Function (ChemUSES)
		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
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

No.	Use Category	No.	Function (ChemUSES)
		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
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

No.	Use Category	No.	Function (ChemUSES)
		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
		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

No.	Use Category	No.	Function (ChemUSES)
		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
		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
		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

No.	Use Category	No.	Function (ChemUSES)
		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 II-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

No.	ChemUSES Function	Use category EU (No.)
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

No.	ChemUSES Function	Use category EU (No.)
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

No.	ChemUSES Function	Use category EU (No.)
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	55

No.	ChemUSES Function	Use category EU (No.)
	agents	
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

No.	ChemUSES Function	Use category EU (No.)
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

No.	ChemUSES Function	Use category EU (No.)
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 II-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 (t/a): □, □ □ □, □ □ □. □ □ □
B Imported (t/a): □, □ □ □, □ □ □. □ □ □
C Exported (t/a): □, □ □ □, □ □ □. □ □ □

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	□ □ □	□ □	□	□	□	□	□	□	□	□	□	□
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 ($\mathbf{F_{ms\text{-}form}}$)	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 8- Guidance document for the use of aquatic model ecosystem studies for biocides

Table of contents

1. Introduction

Authorization of an active substance requires that "*the biocidal product has no unacceptable effects itself, or as a result of its residues, on the environment*" (Article 19, 528/2012/EC) when the product is used according to the intended purpose. The potential ecological risk of the active substance is assessed by a risk assessment. In the first instance, a base set consisting of standard laboratory studies reflecting worst-case conditions is considered using internationally accepted guidelines (OECD, OPPTS). The predicted no-effect- concentration (PNEC) is calculated from the lowest endpoint derived from such standard acute or chronic laboratory tests using an appropriate assessment factor. The PNEC is compared to the predicted environmental concentration (PEC), which itself is based on realistic worst-case assumptions. In cases where the PEC/PNEC ratio is below 1, the risk is considered acceptable due to the margin established between the concentration at which no relevant ecotoxicological response is expected and the realistic worst case exposure concentration predicted from the biocidal use. In cases where the ratio is above 1, there is insufficient confidence for the absence of unacceptable effects and, an authorisation would require further investigations aiming to render more precisely the predicted no-effect-concentration and/or the expectable exposure situation for the ecosystem of concern. Well designed and scientifically based non-standard refined aquatic studies are considered to be a suitable instrument to derive a more realistic PNEC.

The TGD (2003) provides only very limited guidance on how to design and employ aquatic model ecosystem studies. This resulted in a range of different assessment approaches by the various Member States and a heterogeneous treatment of biocidal active substances. A harmonized approach is required including a need to transfer knowledge and experience as available for other legislation considering the special situation of biocides.

In the registration procedure of plant protection products in the framework of Regulation 1107/2009/EC (replaces Directive 91/414/EEC) aquatic model ecosystem studies, usually referred to as mesocosm studies, are used more frequently to derive refined regulatory acceptable concentrations (RAC). For the assessment of plant protection products extensive research has been conducted and guidance documents have been issued discussing test design and interpretation of non-standard studies (e.g. CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999 and ELINK edited by Brock et al. 2010a, draft guidance document on tiered risk assessments for plant protection products, EFSA 2013). In addition, guidance was given for the setting of Environmental Quality Standards published under the Water Framework Directive (2000/60/EC) in which information for the use and design of non-standard studies for refinements is available (TGD EQS 2011). In addition more specific guidance is available on Member State level (Brock et al. 2011).

The integration of methods and decision schemes developed under other legislation will help to foster harmonization for biocides. This can help to generate consistent refinement approaches for the aquatic risk assessment.

The guidance presented here is seen as an extension of the TGD (2003) as it gives further guidance. It is as such intended to supplement the TGD. The approaches outlined in this document are mainly related to the refinement of the risk assessment for parent compounds, but can also be extrapolated to metabolites. The focus of this document is refinement for the $PNEC_{water}$ but general principles can also be applied for the derivation of the $PNEC_{sediment}$.

2. Regulatory background and general principles

Member States must only authorize a biocidal product if the product or its residues have no unacceptable effects on the environment. Biocides are divided into different product-types representing different uses. The requirements for the environmental risk assessment are listed in the Annexes of Regulation 528/2012/EC. The available data for different substances can vary considerably. Generally, minimum testing requirements for the aquatic risk assessment comprise a base set of single-species short-term studies for fish, *Daphnia* and algae. For most product-types, the base set is extended by chronic studies with these standard species. It is commonly agreed that these studies are conducted according to international accepted guidelines (OECD, OPPTS). The technical guidance document (TGD, 2003) gives advice on testing strategies in cases where the data package is incomplete.

For active substances that are also registered as a plant protection product under Directive 91/414/EEC which is replaced by Regulation 1107/2009/EC much more comprehensive data packages are often available.

The lowest (most sensitive) endpoint is divided by an appropriate assessment factor to derive the PNEC. The size of the assessment factor reflects the uncertainties regarding:

- variation of toxicity data within and between laboratories;
- the variation within and between species;
- potential chronic effects in cases where only acute studies are available and;
- the extrapolation from laboratory to field conditions.

In the TGD (2003) standard assessment factors are established for acute and chronic endpoints available for the different compartments of concern. As the uncertainty is reduced the more data are available, the lower the assessment factor is to be considered, e.g. when long-term toxicity data are available from three species across three trophic levels the assessment factor is reduced to 10, provided that the potentially sensitive species groups are presented in the dataset. Moreover, data on the toxicity to other organisms than the standard species representing as such different trophic levels, taxonomic groups, traits or feeding strategies broaden the knowledge on the substance to be assessed and justify the reduction of the assessment factor.

In the risk assessment, exposure concentrations (i.e. PECs) are divided by the effect concentration (i.e. PNECs) to determine the risk. If the PEC/PNEC ratio is > 1 a potential risk is indicated and refinement of the risk ratio would be required to show a safe use. As such, the refinement can be based upon the further analysis of the PEC on the one side as well as of the ecotoxicological response, the PNEC, on the other side.

For the calculation of PECs, standard approaches considering conservative assumptions are provided by straightforward emission scenarios. The exposure estimation considers the release rate of biocides originating from its use pattern. All potential emission sources and the releases to the receiving environmental compartment(s) as well as the fate of the substance need to be analyzed.

There is some uncertainty how more elaborate data (e.g. field studies) can be used. For communication of potential risks harmonized evaluations across different legislation - some of them assessing the same chemical - are crucial. Therefore, agreement on experiments that can be used to generate input data for models or to

refine default values in emission scenario documents are needed as well as refined approaches in modelling require definition as it is done in other areas where chemical risk assessments are performed. For some product-types refined modelling approaches have been developed (e.g. PT8 wood preservatives) but more effort is still needed in this area. Further, the refinement of the release from sewage treatment plants (e.g. elimination studies according to OECD 303a) will in addition help to gain a more realistic impression of exposure. Refinements of PECs by more sophisticated exposure scenarios, however, are not discussed in the context of this document.

The risk assessment performed with base set data is (by design) conservative and so refinements are needed for when a substance do not pass the standard risk assessment. In principle the PEC/PNEC ratio can be refined by:

- using refined toxicity endpoints e.g. from species sensitivity distributions, mesocosm (field) studies etc.;
- using refined emission scenarios.

Goal of all refined risk assessments is that the uncertainty is reduced through an increased amount of information leading to a consistent and meaningful ecotoxicological endpoint that can be used for regulatory purposes. Ecotoxicological observations from tests performed under more representative environmental conditions than standard laboratory tests add on the understanding about the substance of concern respective substance as do further data on other species than the specified base set. In the TGD (2003) guidance is given on the use of species sensitivity distributions (SSD) while other refinement options are not sufficiently addressed. However, other refinement possibilities are available and guidance is needed on how these can be incorporated into current practice. The obvious examples are model ecosystem studies. These experiments that improve the understanding of the ecological response of the aquatic community to a chemical have been found a highly valuable tool in the registration of plant protection products and ample of guidance is available (CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999, OECD, 2006 and ELINK edited by Brock et al. 2010a).

When a model ecosystem study is needed for the refined assessment it is important that the approach follows the identified area of concern from the assessment of the base set data. The expected exposure profile as well as specific characteristics of the compound (e.g. physical and chemical properties, mode of action on targeted and non targeted organisms, toxicological profile) must lead the test design in order to clarify fields of uncertainty and relevance for the risk assessment.

The final risk assessment should be based upon the overall weight of evidence considering and interpreting all the different lines of evidence (e.g. a laboratory test, a field experiment, an observational field study, information from similar compounds) (see Suter and Cormier, 2011).

3 Model ecosystem studies

3.1 General aspects

3.1.1. Introduction

Model ecosystem studies (in this context referred to as mesocosm studies) are a valuable tool to study effects of chemicals with a greater environmental realism. Mesocosm "*are bounded systems that are constructed artificially with samples from,*

or portions of, natural aquatic ecosystems, or that consists of enclosed parts of natural surface waters. They usually are characterized by a reduction in size and complexity when compared with their natural counterparts but they include an assemblage of organisms representing several trophic levels" (EFSA, 2013, page 110). Temperature, light or pH that influence the population dynamics in the ecosystem are naturally established in the test and provide as such a vital base for the responses to the chemical stressor. In contrast to single species tests, semi-field mesocosm and field studies allow for the assessment of a higher number of species and ecological groups, species interactions and secondary effects, endpoints that reflect a higher level of biological organization. Since these studies are performed for a relatively long time also latency of effects can be covered. Limitations of mesocosm studies are a limited number or absence of long-living species as compared to field communities (Beketov et al., 2008) and partly the limited consideration of indirect effects (Von der Ohe et al., 2011).

Information gathered from mesocosm studies can help to minimize the impact on community structure and consequently, ensure long-term functioning of aquatic ecosystems (Figure 8-1).

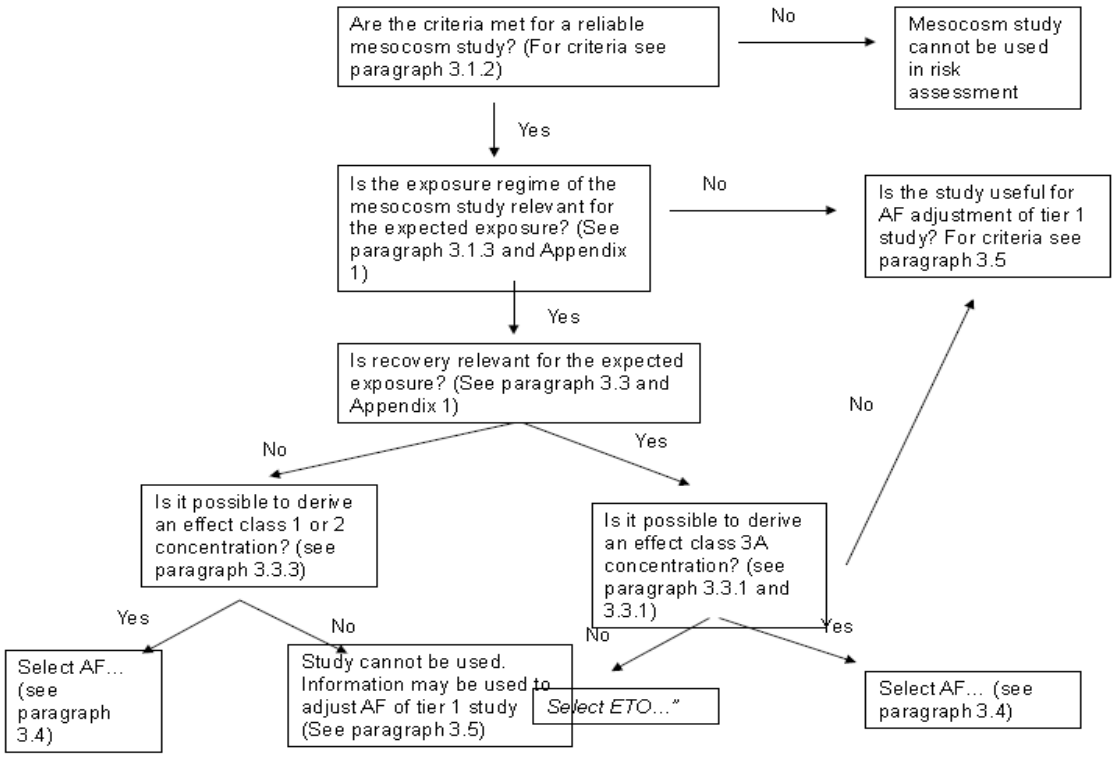


Figure 8-1. Decision scheme depicting the different assessment steps of a mesocosm study

3.1.2. Criteria for reliability

Based on the general principles of reliability assessment by Klimisch et al. (1997), De Jong et al. (2008) developed extensive guidance on the evaluation of mesocosm studies, which of course can also be seen as guidance for designing and reporting new studies. The following questions should be answered when assessing the quality of the study:

1. Is the test system adequate and does the test system represent a relevant freshwater community?
2. Is the description of the experimental set up adequate and unambiguous?
3. Is the exposure pattern adequately described?
4. Are the investigated endpoints sensitive and in accordance with the working mechanism of the compound?
5. Is it possible to evaluate the observed effects statistically?

Only studies which fulfill these reliability criteria should be used in the assessment. Some of the aspects are further elaborated on below.

EFSA (2013) deals with effects on freshwater ecosystems only, and existing mesocosms performed for PPP authorization address freshwater systems. Little information is present on the representativeness of these studies for marine risk assessments. Differences in pH, salinity, (sensitive) taxa, water refreshment due to tidal exchange, etc., may all contribute to differences in results. It is therefore advised not to use freshwater mesocosm studies as a basis for a marine risk assessment, and vice versa, unless there is scientific evidence that the ecotoxicological response in both types of systems is comparable.

3.1.3 Representative aquatic community

Mesocosm studies should address the potential effects on sensitive species or species groups in a full community. A sufficient number of representatives of taxonomic groups or species with representative biological traits should be present in the test system to provide a result of improved ecotoxicological relevance. Particularly taxa which are expected to be sensitive to the mode of action of the tested substance should be included, e.g. algae and macrophyte species in a study with an herbicide that inhibits photosynthesis, or insects for insecticides. For plant protection products it is specified that "*at least 8 different populations of the sensitive taxonomic group need to be present*" (EFSA, 2013, page 113). This criterion can be transferred to biocides. A number of biocidal actives will have a broader range of potentially sensitive taxa, and similar to EFSA's advice for fungicides, this should be accounted for by including a wider range of non-vertebrate taxa in the mesocosm design. Therefore, in cases where recovery is considered for risk assessment (see 3.1.5 below) it has to be carefully evaluated if potentially vulnerable taxa (e.g. uni- or semivoltine invertebrates with a low dispersal rate and/or macrophytes with a slow growth rate) are sufficiently represented, because recovery of these taxa will be slower than for species with a short life-cycle. The intrinsic sensitivity of insects is not correlated with voltinism (see e.g. Brock et al., 2010a), and there are no indications that slow-growing macrophytes are consistently more sensitive than e.g. algae, but sensitive multi-/bivoltine insects recover faster from insecticide stress than sensitive uni-/semivoltine insects (e.g. Van den Brink et al., 1996; Brock et al., 2009; Liess and Von der Ohe, 2005). In cases where recovery is not considered for risk assessment (indicated as the "ecological threshold option" (ETO)), the (in)ability to recover is not an issue because effects are not accepted at all. EFSA (2013) states

that "it needs not to be a problem when sensitive univoltine and semivoltine invertebrates with low dispersal ability or macrophytes with a relatively slow growth-rate are not sufficiently represented in the test systems. Instead, the availability of data on negligible effect concentrations for species sensitive to plant protection products […] may [be] suffice to derive an ETO [= environmental threshold option] - RAC"(EFSA, 2013, page 113). A similar reasoning would apply to biocides.

3.1.4 Exposure

For the design of new studies as well as for the evaluation of existing ones, insight into the predicted exposure profile (PEC-profile, the development of predicted concentrations over time), is a prerequisite for the use of mesocosm studies for risk assessment. For a straightforward risk assessment, the exposure profile in the mesocosm should be relatively worst case as compared to the PEC-profile in the water body. If exposure in a mesocosm study has been shorter or involved lower concentrations than expected for the proposed use, absence of effects in the mesocosm experiment cannot be used directly to demonstrate that no unacceptable effects will occur in the field situation. To illustrate this, some hypothetical cases are presented below. In Figure 8-2, on the left hand side, the situation is plotted in which initial exposure in the mesocosm is higher and concentration decline is slower than predicted for the proposed use. Still, no effects are observed in the mesocosm, which may be used as an indication that the proposed use will not lead to unacceptable effects. On the right hand side, the opposite situation is plotted: no effects are observed in the mesocosm, but the proposed use results in a higher peak and longer presence of the substance than considered in the mesocosm.

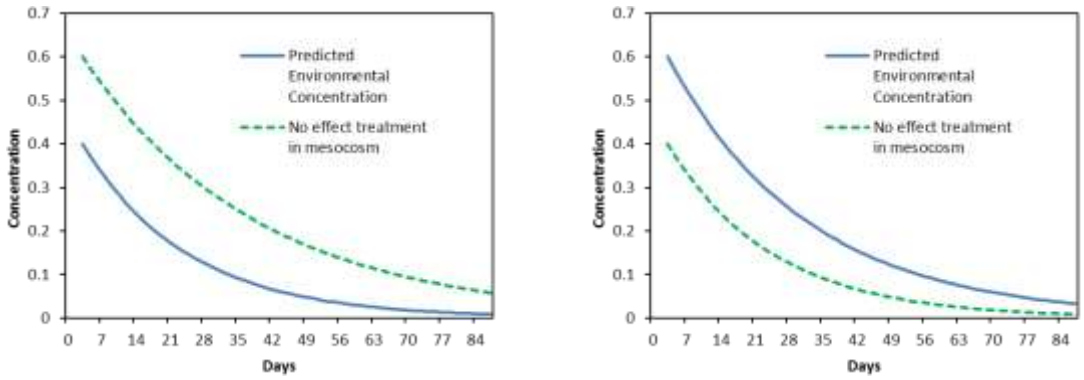


Figure 8-2: Comparison of the exposure profile in the mesocosm with the predicted exposure for the proposed use. Left: mesocosm is worst case for PEC. Right: mesocosm is best case for PEC.

Figure 8-3 shows a more complicated situation. On the left hand side, no effects are seen in the mesocosm with a peak concentration that is higher than predicted for the proposed use, but decline in the mesocosm study is faster than in the field. On the right hand side, the initial concentration in the mesocosm is lower than predicted for the proposed use, but the substance has been present in the mesocosm for a much longer time than predicted in the field. In these cases, it is not clear beforehand whether or not the mesocosm represents a worst case. If effects of the substance result from initial exposure during the first days, the mesocosm treatment with a higher initial peak might still be worst case, even if decline later on is faster. If, however, effects are due to prolonged exposure, the difference in decline rate may become more important. In these cases it should be considered if the concentration

related to the NOEC-treatment when described in terms of a time weighted average concentration can be used for risk assessment. Further guidance on this is provided in the next chapter.

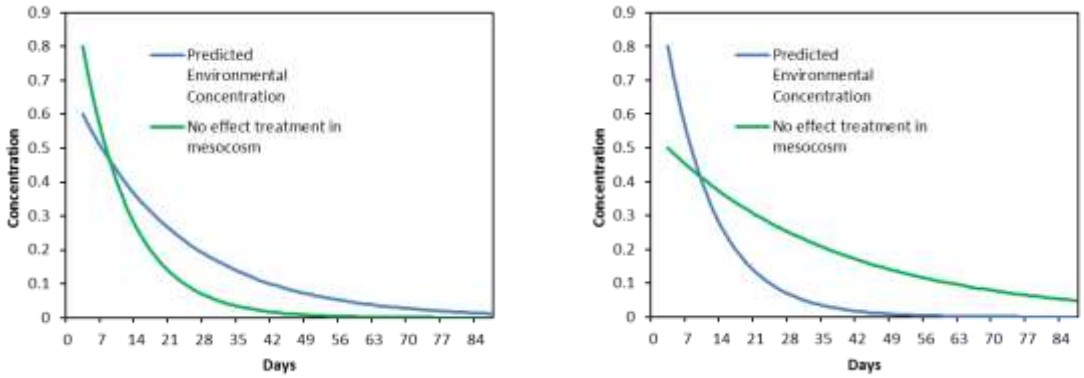


Figure 8-3: Comparison of the exposure profile in the mesocosm with the predicted exposure for the proposed use. Left: mesocosm is worst case for PEC when considering the peak, but not with respect to concentration decline. Right: mesocosm is not worst case with respect to initial exposure, but the substance has been present for a longer period of time without showing effects.

From these examples, it is clear that knowledge of the PEC-profile is essential both for designing new studies, and to evaluate whether or not an existing mesocosm can be used for the assessment of a different use. It is expected that for biocides authorisation the latter issue is particularly important, since a number of biocidal active substances have already been marketed as plant protection products. The focus of existing studies will often have been at simulating the predicted exposure resulting from plant protection product use, which is characterised by time-variable concentrations (EFSA, 2013). Typical profiles resulting from exposure modelling used for plant protection product assessment are characterised by repeated pulses. The height and duration of the peaks, and the interval between them will depend on agricultural practice, physico-chemical characteristics of the plant protection product, the relative importance of the different routes-of-entry (e.g. drift, run-off, drainage) and the characteristics of the water body (EFSA, 2013). In contrast, for the majority of biocides, predicted exposure will be constant because the emission scenarios consider daily use, discharge to a STP and daily emissions of the STP to the receiving water body. This puts special demands on the mesocosm design, although it does not necessarily mean that only mesocosm studies with constant exposure can be used for risk assessment. Further guidance on this is provided in Sections 3.2 and 3.3 of this Guidance. Some PTs may result in non-continuous exposure, i.e. distinct peaks or in some cases irregular peak patterns comparable to those of plant protection products. A summary is given below in Table 8-1. No ESDs are available for PT 16, 17, and 20, and a draft is available for PT 19. These PTs are therefore not included in the table. Table 8-4 Overview of emission patterns per product-type gives a more detailed overview of the expected exposure patterns per PT in order to facilitate the design and evaluation of the mesocosm studies. Note that Table 8-1 and Table 8-4 are meant as a generic overview, and the profile of a specific case may be different. As indicated above, it should always be checked whether the mesocosm study adequately represents the exposure profile resulting from the biocide use. Ihose PTs where emission is indicated as "potentially not continuous", a

careful examination of the expected exposure profile is needed to decide on the relevance of the mesocosm design for a particular intended use.

Table 8-1: Summary of expected exposure patterns for biocide product–types (PT between brackets: probably only in specific cases).

Continuous emissions	Potentially non-continuous emissions
PT 1, 2, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15, 21	(2), 3, (9), 11, 12, 18

3.1.5 Evaluation of endpoints and acceptability of recovery

In order to draw meaningful conclusions from a mesocosm study it is important that the appropriate endpoints are measured in a sufficient frequency to cover the specific protection goal. The protections goals for biocides have only been phrased in general terms but at present biocide risk assessment generally considers the population in the case of aquatic algae, vascular plants and invertebrates, individuals to populations in the case of vertebrates and populations to functional groups in the case of aquatic microbes. "*This implies that for most organisms at risk that are studied in micro-/mesocosm tests the selected measurement endpoints should relate to relevant population-level endpoints, more specifically the attributes survival/growth and abundance/biomass*" (EFSA, 2013, page 115). To study community level responses, multivariate analyses, parameters like diversity indices as well as endpoints indicative for community processes like dissolved oxygen are recommended. The assessment of reliability of a mesocosm study is described in detail by De Jong et al. (2008) and EFSA (2013). A critical part of the evaluation of mesocosm studies is the statistical analysis of measurement endpoints related to effects. Various univariate and multivariate techniques are available for evaluation of effects at the population and at the community level, to calculate NOECs and LOECs. To ensure that an effect is treatment related and not background variability, information about the statistical power of the NOEC/LOEC values is required. Therefore, EFSA (2013) advises that the minimal detectable difference (MDD) is reported for each measurement endpoint. Calculating the minimal detectable difference (MDD) allows reporting the actual effect which could be determined in the experiment for a given endpoint at a given time. A high MDD means that large changes are not detected as significant, due to e.g. variability in the control or low abundance. For applying the MDD concept to mesocosm experiments it is noteworthy that the MDD is particularly important if no effect is observed, since when a LOEC can be calculated the statistical power apparently is high enough to detect an effect. EFSA (2013) states that the MDD should preferably be lower than 70-90%. However, EFSA (2013) also requires that for at least 8 sensitive taxa a statistical evaluation of the dose-response relationship should be possible, meaning that the MDD should be sufficiently low. The case study with an insecticide that is included in the EFSA guidance shows that indeed low MDDs for sensitive endpoints are possible.

The identification of treatment related responses should not be based on statistical evaluations only, but also on ecotoxicological and ecological knowledge. Single species laboratory data can help to put results of a mesocosm study into perspective and can be considered along with the results from the mesocosm studies. De Jong et al. (2008) and the EFSA (2013) should be consulted for more guidance on statistical analysis and the MDD.

For the reason of a better comparability of studies and their interpretation for the protection level to be achieved, Effect classes as described by de Jong et al. (2008)

and adapted by EFSA (2013) should be used to evaluate effects (Table 8-2). For further details, reference is made to the original report (de Jong et al. 2008) and the PPP guidance by EFSA (2013).

Table 8-2: Definition of endpoints of mesocosm studies. Classification into Effect classes according to EFSA (2013)

Effect class	Description
0	*Treatment related effects cannot be evaluated*. Due e.g. low abundance and variability the MDD was always larger than 100 % so even very strong effects could not be determined for the endpoint evaluated. If this class is consistently assigned to endpoints that are deemed most relevant for the interpretation of the study, the regulatory reliability of the micro-/mesocosm tests is questionable.
1	*No treatment-related effects demonstrated for the most sensitive endpoints*. No (statistically and/or ecologically significant) effects observed as a result of the treatment. Observed differences between treatment and controls show no clear causal relationship.
2	*Slight effects* Effects concern short-term and quantitatively restricted responses usually observed at individual samplings only.
3A	*Pronounced short-term effects (< 8 weeks, followed by recovery)* Clear response of endpoint, but full recovery of affected endpoint within 8 weeks after the first application or, in the case of delayed responses and repeated applications, the duration of the effect period is less than 8 weeks and followed by full recovery[17]. Treatment-related effects demonstrated on consecutive samplings.
3B	*Pronounced effects and recovery within 8 weeks post last application* Clear response of the endpoint in micro-/mesocosm experiment repeatedly treated with the test substance and that lasts longer than eight weeks (responses already start in treatment period), but full recovery[17] of affected endpoint within eight weeks post last application.
4	*Pronounced effect in short-term study* Clear effects (e.g. large reductions in densities of the population) observed, but the study is too short to demonstrate complete recovery within eight weeks after the (last) application.
5A	*Pronounced long-term effect followed by recovery* Clear response of sensitive endpoint, effect period longer than 8 weeks and recovery did not yet occur within 8 weeks after the last application but full recovery[17] is demonstrated to occur in the year of application.
5B	*Pronounced long-term effects without recovery* Clear response of sensitive endpoints (> 8 weeks post last application) and full recovery cannot be demonstrated before termination of the experiment or before the start of the winter period.

The endpoint (NOEC) from a mesocosm study to be used for biocides risk assessment should preferably be derived on the basis of the treatment that is classified as Effect class 1. However, since Effect class 2 refers to slight effects that are observed on a single occasion, this Effect class might be used also to derive a NOEC from a mesocosm study. Moreover, when more measurement endpoints are assessed on several sampling days (which usually is the case in micro-/mesocosm experiments) that the chance of occurrence of Type II statistical errors may increase (demonstrating a statistical difference when there is not a treatment-related effect). For this reason it could be decided that a single Effect Class 2 response could be seen as the NOEC of the study (Brock et al., 2011), but a higher assessment factor may be applied.

[17] An endpoint is considered as recovered if the MDD allows statistical evaluation during the relevant recovery period (so excluding MDD class 0) and the conclusion of no statically significant effect between treated systems and controls is not caused by a decline of that endpoint in controls (e.g. at the end of the growing season). If these criteria are violated a higher effect class has to be selected.

The recovery option is not applicable to product-types that result in continuous exposure. In case biocide emissions lead to a short-term peak on only few occasions during the year e.g. meeting the definition of intermittent release according to the TGD (2003), considering the recovery option might be reasonable. The potential for recovery should be judged in relation to the product specific exposure pattern (Appendix 1). Thus, it has to be thoroughly checked if the expected exposure pattern allows for recovery. In the light of harmonization and for registration of active substances on a European level, Effect class 3A endpoints are used for the ecological recovery option. If the PNEC is based on a mesocosm using an Effect class 3A endpoint, special attention should be paid to the representativeness of potential sensitive populations. It is suggested to link the PNEC and the respective covered biocidal use in the list of endpoints. Additional data in relation to the use pattern can be submitted at product authorization stage. Note, that for product authorization on MS level different time periods for recovery might be acceptable (e.g. reduced recovery time in colder areas like in some Nordic countries).

In summary, the results of a properly designed and conducted mesocosm study can thus be used in the effect assessment in two ways (Figure 8-4):

- by accepting no (or only negligible) population effects (ecological threshold option) or;
- by accepting some population level effects if ecological recovery takes place within an acceptable time period (ecological recovery option); only acceptable if exposure pattern allows for this option.

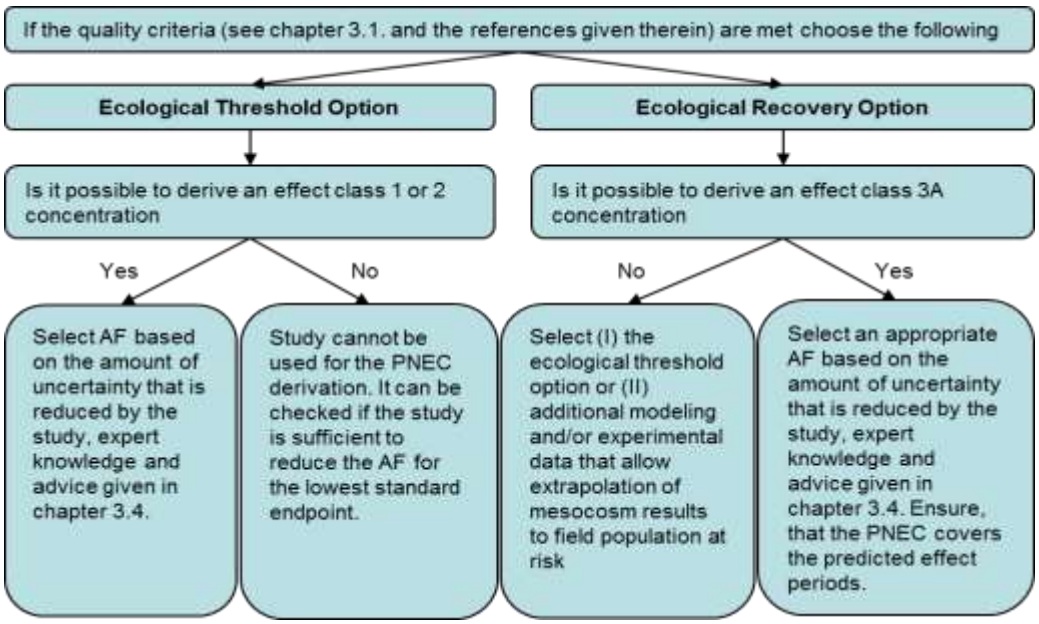


Figure 8-4: Decision scheme for the derivation of PNECs based on mesocosm studies (EFSA, 2013, page 124; adapted)

3.2 Design of new studies

For the design of mesocosm studies, guidance is given by OECD (2006), EFSA (2013) and in various workshop documents and publications (e.g. CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999, ELINK edited by Brock et al. 2010a and de Jong et al. 2008) and will not be repeated in detail in this document. In addition to the references given above, the main points given in

chapter 3.1 and aspects that are particularly important for biocides should be considered for the design of new studies.

The dose selection should be based on results of the base set data and known effects from literature. Special attention should be given to the anticipated exposure pattern in the field (i.e. the predicted PECs, see 3.1.4 above) and to the question whether recovery can be taken into account or not (see 3.1.5 above). Information from structurally similar compounds can help to properly design the study if the used information is relevant and reliable. Studies which have been peer-reviewed under European or national legislation are a valuable data source. For substances reviewed under Directive 91/414/EEC (replaced by Regulation 1107/2009/EC), the exposure pattern, particularly from tailor-made studies, will often not reflect the exposure pattern resulting from biocidal uses. Nevertheless, these studies can be considered as they provide valuable information, for example on the distribution of sensitivities among species or groups of species.

The active substance should be preferably used as test item. However, for some substances this might not be practicable (e.g. too low water solubility of the active substance). In these cases a formulation may be used as test item. The chosen formulation is preferably the biocidal product that is planned to be authorised. Although a formulation contains several substances, the effects are usually driven by the active substance. In cases for which the tested formulation is not equal to the biocidal product information should be provided to show that the toxicity of the formulation is comparable to the active substance.

Depending on the properties of the active substance it has to be kept in mind that test organisms are exposed to the parent compound as well as to metabolites if these metabolites are stable for a certain time. An appropriate analytical analysis should be conducted so that an assessment of both the exposure and effects of any relevant metabolites can be made. Therefore, if a higher tier study is commissioned and relevant metabolites have been identified in fate and behaviour studies, these metabolites should be measured in order to include them in the risk assessment

3.3 Evaluation of already available mesocosm studies for biocides

A concept for the re-evaluation of mesocosm studies which were conducted for purposes other than the support of a biocidal registration authorisation (i.e. typically for plant protection products) is developed on the basis of different exposure patterns. In such cases it is important to determine which part of the exposure is most relevant in terms of ecotoxicological effects leading to the ecotoxicologically relevant concentration (ERC).

There are three different kinds of exposure:

- single peak (see 3.3.1 below),
- multiple peak (see 3.3.2 below) and
- continuous exposure (see 3.3.3 below).

As explained in Section 3.1.4 of this Guidance above a decision should be made whether or not the mesocosm adequately represents the exposure profile resulting from biocide use.

Before listing the recommendations, a general point havehas to be addressed: effect concentrations can either be expressed as nominal or initial measured or as time-weighted-average (TWA) concentrations. If the TWA approach is used, particular attention should be paid to the time interval over which the TWA is calculated. The

time window for the TWA is not necessarily identical to study duration of the mesocosm nor to standard tests in the laboratory, instead it is driven by the ecological response time and the duration of the exposure in the study.
It is important to get an understanding of the exposure phase that is most relevant for inducing toxic effects (Brock et al. 2011). The pragmatic approach to base the TWA on the length of the chronic study that triggered the risk was proposed by Brock et al. (2011) in a Dutch national guidance for the derivation of long-term environmental standards. This approach is also used by EFSA (2013) and is seen as being "*most likely being relatively worst case*" (EFSA, 2013, page 49). If scientific data are available that demonstrate that another TWA is more appropriate e.g. information on the ratio between acute and chronic effects, the time to onset of effects or the length of the most sensitive life stage of the organisms at risk, the time window should be shortened or lengthened. If there is reasonable concern that the TWA based on the chronic study that triggered the higher tier study is too short, e.g. if effects in the mesocosm last longer than the duration of the critical chronic laboratory study, it is proposed to base the length of the TWA on the time span during which the most sensitive species in the mesocosm is affected, i.e. from the onset of effects until recovery. This period is derived from the treatment above the NOEC, i.e. above Effect class 2 (see figure 8-5) (NOEAEC for plant protection products). This time window is then used to calculate the TWA concentration from the NOEC treatment. In case multiple species are affected then the longest time window should be taken as a basis for the TWA calculation. This approach is only applicable if the mesocosm involves a treatment with recovery of effects within the duration of the study.

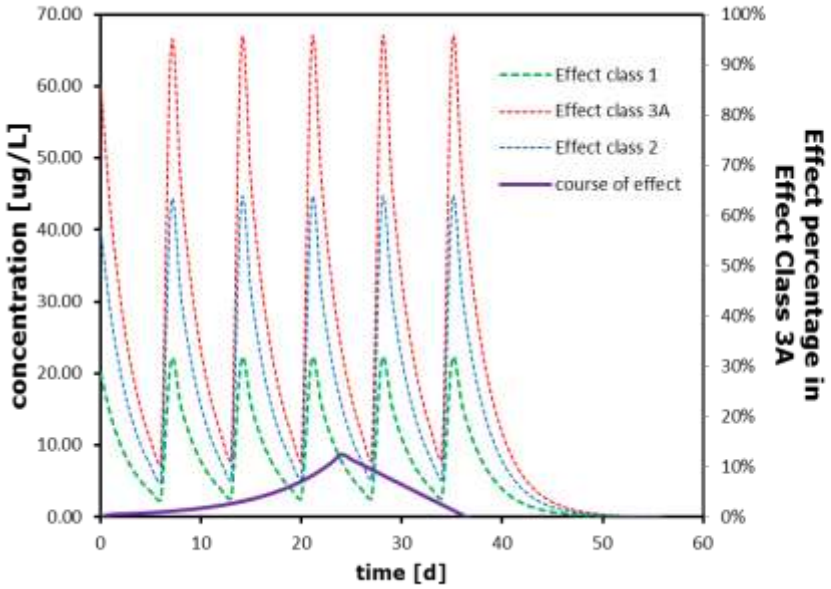


Figure 8-5: Representation of mesocosm treatments with Class 1, 2 and 3A effects (dotted lines, primary vertical axis) and time course of effects in Effect Class 3A (purple line, secondary vertical axis).

In the eventual case that a reliable mesocosm study cannot be used directly to derive the $PNEC_{water}$, e.g. because the exposure regime is not adequate, it nevertheless needs to be evaluated as the additional information adds on the

knowledge of the overall toxicological profile of the compound of concern. For example, mesocosm studies may point at the sensitivity of a taxon that was not included in the laboratory dataset, or mesocosm studies can confirm that a taxon is apparently non-sensitive. Mesocosm data may thus confirm that testing of additional taxa will likely (not) result in lower endpoints. They may reduce the uncertainty when statistical extrapolation methods are applied to laboratory data (Species Sensitivity Distributions (SSD)). This may be a reason to adapt the assessment factor used on laboratory data. It should be realized, however, that when a mesocosm is considered not suitable for PNEC-derivation because the exposure is not relevant for the predicted field exposure, care should be taken when deciding on adapting the assessment factors for a chronic risk assessment based on laboratory studies. In addition, a mesocosm that is judged as not suitable for the surface water risk assessment might still provide useful information for the sediment risk assessment.

3.3.1 Single peak exposure

For studies with single peak exposure, the dissipation time of the substance in water is the first decision criterion.

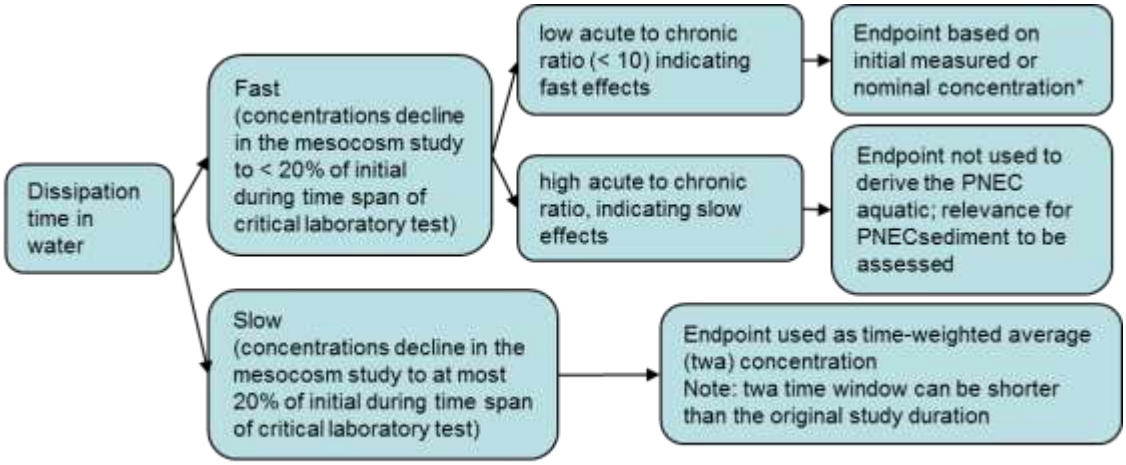


Figure 8-6 Assessment scheme for single peak exposure studies

For non-continuously released biocides, the initial peak in the treatment which resulted in Effect Class 1 or 2 can be used directly if the peak and decline rate in the study is worst case as compared to those for the field, i.e. if the peak in the mesocosm is higher and the DT_{50} for dissipation from the water phase long enough to cover the exposure that is predicted for the field (see Figure 8-2, left hand side). When the initial concentration is used for the effects assessment, the PNEC should be compared with the $PEC_{initial}$.

For continuous exposure, it should be judged whether the exposure in the mesocosm study has been long enough to consider the study relevant for the derivation of the PNEC for long-term exposure. For this, Brock et al. (2011) propose that test concentrations between peaks should not decline to <10% of initial. EFSA (2013) gives a more strict criterion for the use of a single pulse mesocosm study for chronic risk assessment, and requires a maximum decline to 20% of initial (i.e. <80%

decline) within the time window relating to the duration of the test that triggered the risk assessment. This can be judged from the reported concentrations or using the dissipation time. The minimum required dissipation time can be calculated from the formula $C(t) = C(0) \cdot e^{(-kt)}$, where C(t) is the concentration after t days, C(0) is the initial concentration, k is the decline rate constant and t is the duration of the critical laboratory test.

If the dissipation time in the mesocosm is faster and leads to <20% of initial remaining after the critical time, the acute to chronic ratio (ACR) may be considered. For the calculation of the ACR the ecological group that triggered the mesocosm study is used. For substances with a lower ACR (i.e. < 10) which show a short time-to-onset-of effect, the endpoint can be expressed as the initially measured concentrations or the nominal concentration. Nominal concentrations are used if the measured concentration is between 80-120% of the nominal. Mesocosm studies with substances which dissipate fast but also have a high ACR, indicating that effects assessment is driven by longer/constant exposure, cannot be used directly for the derivation of the $PNEC_{water}$. However, these mesocosm studies might be used for the sediment assessment, when the concentration has been measured in the sediments and benthic organisms have been present in the system in a sufficient number. If the substance that disappeared from the water phase is sorbed to sediment, organic matter or organisms it may still contribute to effects that are treatment related. It has to be checked if analytically determined sediment exposure covers field exposure and if the tested species assemblage is representative.

For slowly dissipating substances that meet the criterion of <80% decline of concentrations within the time window of the critical chronic laboratory test the endpoint is based on the relevant TWA concentrations. The time window for the TWA is not necessarily the same as the duration of the mesocosm study (see above).

For instance, Figure 8-7a shows an Effect class 1 mesocosm-treatment where no effects are observed, using a critical study for PNEC derivation for a 21-day chronic daphnid test. In this example, the initial concentration of the active substance is 100 µg/L, and declines with a DT50 is of 9 days. After 21 days the substance has declined to 20 µg/L (green dashed line). This single peak mesocosm study would meet the criteria as described above, for the use of a single pulse mesocosm study for chronic risk assessment. The NOEC of the mesocosm may be calculated as the 21-day TWA (blue dashed line; 50 µg/L), given that the critical 1st tier test is a 21-day Daphnia study, and in the mesocosm treatment level above the highest treatment with no effects, in other words, above the Effect class 1 NOEC, the time to onset of maximum effects was < 21 days. However, in the case where the treatment level above the level identified as Effect Class 1 NOEC, the time to maximum effect would be of 30 days, then the NOEC of the Effect class 1 treatment should be calculated as the 30-day TWA, and in this case the NOEC would be set to 39 µg/L. As a result, by setting the NOEC to 50 µg/L, it is implicitly assumed that continuous exposure at 50 µg/L will not induce effects. In contrast, if the NOEC is not set at 50 µg/L, the assumption is that effects may occur below this level, even in situations where even at higher concentrations than the TWA no effects were observed, as it is the case in this study.

Figure 8-7b shows an example where the critical test conducted is a 28-day insect study, with a slower decline of the substance in the mesocosm system (DT_{50} of 24 days). In this case, and after 28 days, the actual concentration of the substance in the test is 68.5 µg/L. Thus, the criterion of the substance declining a maximum of

80% from the initial concentration is easily met. In this study, the time to the maximum effect is 35 days, and thus in this situation it could be justified to use the 35-day TWA as the basis for setting a NOEC to 62 µg/L.

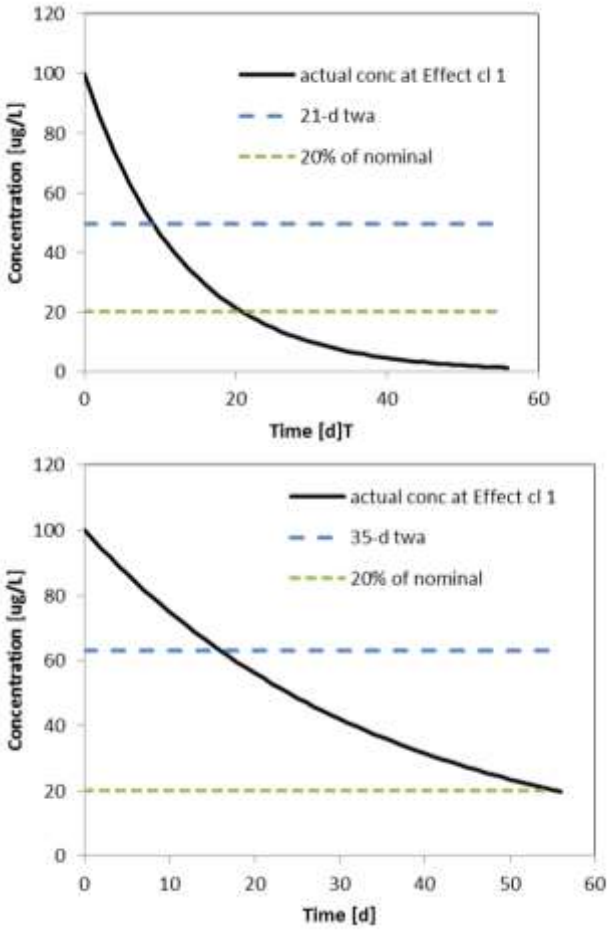


Figure 8-7. Representation of a chronic daphnid study (21 days) in an Effect class 1 mesocosm system for a single peak exposure treatment in situations where the DT50 is 9 days (Fig 8-7a) and 24 days (Fig 8-7b), and where the data can be considered for a chronic risk assessment.

3.3.2 Repeated peak exposure

Repeated pulse studies are considered in a similar way as single pulse studies. If concentrations decline to completely between pulses, the study can in principle not be used for derivation of a PNEC for continuous exposure unless at least 20% of initial concentration is present over the duration used for the TWA time window (if the TWA approach is feasible) of the critical laboratory test. In practice, this will mean that studies, in which concentrations decline completely in between pulses, will be treated as a single pulse study. For rapidly dissipating compounds (i.e. if the DT_{50} of a substance in the mesocosm is shorter than the trigger as calculated above), application has to be repeated before concentrations have dropped to 20 % of initial and application has to be continued until the total application period is long enough to cover at least the duration of the most critical laboratory test.

If a mesocosm study with repeated applications of a fast dissipating compound does not meet the criteria as described above, additional laboratory studies and/or modeling approaches may be used to demonstrate that continuous exposure would not lead to different results than observed in the repeated pulse studies.

For this assessment, results from laboratory studies with a semi-static or continuous design can be compared. For such a comparison, species should be used that are preferably closely related to the sensitive taxon found in the mesocosm. If the endpoints are in a comparable range (factor 3 difference), the endpoint of the mesocosm study can be expressed as a TWA concentration. If the toxicity is not comparable, a further evaluation is needed. This can for example include time-to-event studies or modeling approaches.

Models can provide information on the acute and long-term impacts of substances present over a range of exposure durations and frequencies. Mechanistic effect models may help to integrate the ecological and environmental parameters and thus also increase the understanding of the complex interactions and mechanisms of potential biocide impacts on ecosystems. Toxicokinetic/toxicodynamic models (Ashauer et al. 2011) will help to evaluate the potential long-term impact of non-continuous exposure situations. If modelling approach are used some general rules should be applied across the different models such as 'good modelling practice' and proper documentation of all assumptions, input parameters and modelling steps (Schmolke et al. 2010). An overview of the state of the art with respect to effect modelling, considering toxicokinetic/toxicodynamic modelling, population models, community, food web or ecosystem models, and empirical models can be found in the proceedings of the ELINK-workshop (Brock et al., 2010a). The potential role of ecological population models for pesticide risk assessment and registration was discussed during the LEMTOX-workshop (Thorbek et al., 2010). An EFSA opinion on the use of mechanistic modelling approaches is expected for 2016 (EFSA, 2013).

For repeated peak exposure it is also important to consider the toxicological dependency of these pulses for the life span of the individuals of the sensitive species: If recovery is considered ecological independence (peak intervals are greater than the relevant recovery time of the sensitive populations of concern) has to be evaluated (EFSA, 2013).

Generally, a potential relevance of the study for the sediment risk assessment has to be kept in mind especially for substances that dissipates into sediment and are relatively stable (in) there. An EFSA opinion on sediment risk assessment is expected for 2014 (EFSA, 2013).

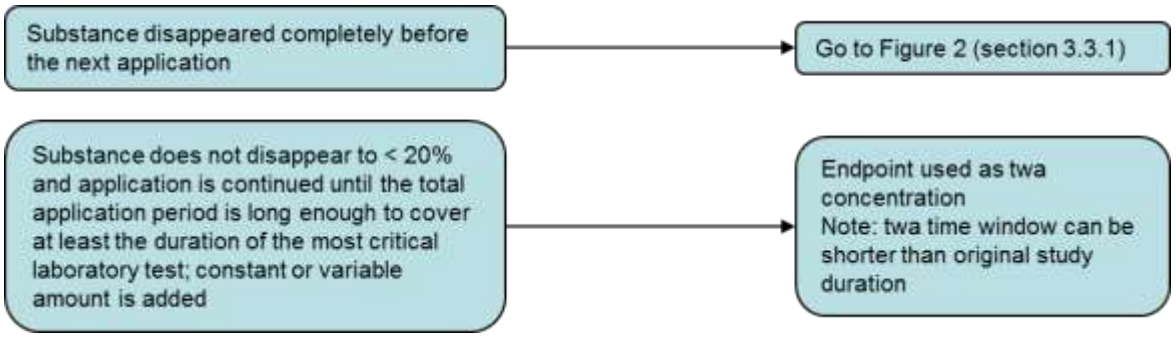


Figure 8-8: Assessment scheme for repeated peak exposure studies

3.3.3. Continuous exposure

As already indicated before, most biocidal PTs will result in continuous exposure. Mesocosm studies with continuous exposure are rather rare, but if present the derivation of a NOEC from these studies follows the same principle as standard laboratory studies. Nominal concentrations can be used if measured concentrations are between 80 and 120 % of nominal, otherwise actual average concentrations should be used.

Whilst the use of a time weighted average approach may be appropriate in some circumstances it always needs to be considered if it is scientifically valid and supported by sufficient evidence to show reciprocity of effects at relevant concentrations and exposure durations

3.4 Application of an assessment factor to derive the $PNEC_{water}$

"*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*" (TGD, 2003 page 93). In the technical guidance document (TGD, 2003) the size of the assessment factor applicable to the endpoint of a mesocosm study is left open. It is only stated that "*the assessment factor to be used on mesocosm studies or (semi-) field data will need to be reviewed on a case-by-case basis*" (TGD, 2003 page 101).

Since mesocosm studies are regarded as an additional step in the risk assessment process which reduces uncertainty, the regulatory trigger values used at assessment of the data from the base set need not necessarily be carried over to the refined risk assessment. Thus, if uncertainty is reduced compared to the preliminary risk characterization, the assessment factor should be reduced.

As stated above the assessment factor has to account for spatio-temporal extrapolation i.e. the mesocosm – field extrapolation. To gain insight into this aspect, Brock et al. (2006) compared the results of mesocosm studies covering ponds, ditches and streams for chlorpyrifos (single peak exposure) and atrazine (multiple peak exposure). Based on endpoints of Effect Class 1 and 2, the spatial and temporal extrapolation of ecological threshold concentrations seems to be possible with relatively low uncertainty. In later work Brock et al. (2008) compared mesocosm experiments in which long-term exposures were simulated and based on these a geographical extrapolation factor was estimated. For their comparison, Brock et al. (2008) used the reported Effect class 1-2 concentrations and calculated the

geometric mean, the range between the lowest and highest reported value, and the 95% confidence limits. The difference between the upper and lower 95% confidence limits, indicated as the spread, was used as a measure of variability. The spread in long-term exposure studies was 1.4 for the surfactant C12TMAC and 5.4 for LAS (surfactant), 1.8 for copper, and 2.5 for atrazine. For short-term pulse studies with chlorpyrifos and lambda-cyhalothrin, the spread was 2.9 and 2.6, respectively. It should be noted that if Effect class 1 and 2 were both reported, Brock et al. (2008) used the geometric mean of these concentrations for their calculations. In an update, the assignment of Effect classes for the atrazine experiments was slightly revised and data for chlorpyrifos, azinphos-methyl, esfenvalerate, simazine and carbendazim were added (see Brock et al., 2011, Appendix 1; EFSA, 2013; Appendix E). Based on this scientific information, it appears that variability in studies is limited when comparing Effect class 1-2 concentrations, variation between studies increases when higher Effect classes are included in the analysis. The NOEC of a well performed mesocosm study (see 3.1.1) is valid for different local and climatic situations and it was concluded by EFSA (2013) that for short-term pulse studies, a small factor may be sufficient to address remaining variability at the level of Effect Class 1-2. For chronic studies, a factor of 2-3 would be sufficient to ensure that the Effect class 2 concentration in a single study does not overlap with higher Effect classes in other studies. For higher Effect classes, a higher factor may be needed to account for the variability between studies in case only a single mesocosm endpoint is available.

Assessment schemes and approaches for the size of the assessment factor are available under different European legislation (see Table 2). Annual average water quality standards (AA-EQS) as determined under 2000/60/EC are intended to protect water organisms against the occurrence of prolonged to continuous exposure. In the TGD EQS (2011) a rather general approach is presented, and regarding the assessment factor it is stated that "where there is (a) only a single model ecosystem study, and (b) sensitive taxa are included in the study of a compound with a specific mode of action, an assessment factor of 5 would account for variation in the NOECs" (EQS TGD, 2011, page 63). Based on the above presented comparison of mesocosm studies for different types of plant protection products and exposure patterns, EFSA (2013) uses lower assessment factors of 2 to 3 and differentiates between Effect class 1 and 2 for derivation of the RAC. For their justification of assessment factors for the AA-EQS Brock et al. (2011) pointed to the fact that, regulatory acceptable concentrations as determined according to EFSA (2013) are intended to protect water organisms in edge-of-field surface waters. Due to the application pattern of plant protection products the focus is on short-term pulses to prolonged exposure allowing in certain cases recovery of populations. Brock et al. (2011) argue that since EQS values apply to a wider range of water body-types, a higher assessment factor is needed for EQS-derivation. Brock et al. (2011) used the above presented comparison of mesocosm studies, and propose assessment factors of 2 to 4 for Effect class 1, and 4 to 5 for Effect class 2.

Table 8-3: Assessment factors for a single mesocosm study as proposed under 2000/60/EC and 1107/2009/EC

Effect class	Assessment following Water framework Directive (2000/60/EC)		Regulation of plant protection products (1107/2009/EC)
	(TGD EQS, 2011)	Dutch PPP guidance, (Brock et al., 2011)	(EFSA, 2013)
1: No treatment	annual average AA-	2 – 4 [2)]	2 [3)]

related effects	EQS: 5 [1)]		
2: Slight and transient effects		4 – 5 [2)]	2 - 3 [3)]
3A: Pronounced short-term effects; recovery within 8 weeks after first application or total period of effects < 8 weeks	Not applicable	Not applicable	3 - 4 [3)]

Notes on Table

"where there is (a) only a single model ecosystem study, and (b) sensitive taxa are included in the study of a compound with a specific mode of action, an assessment factor of 5 would account for variation in the NOECs" (EQS TGD, 2011, page 63). No guidance is given as to whether Effect class 2 may be used for NOEC derivation.

1) "The height of the AF [= assessment factor] is based on expert judgment considering all available lower and higher-tier information. If several adequate micro-/mesocosm studies are available the AF is applied on the highest Effect class 1 or 2 value or a lower AF than reported in the table may be applied" (Brock et al., 2011, page 104).
2) "If several adequate micro-/mesocosm studies or other adequate higher tier studies (e.g. monitoring, relevant population experiments or modelling) are available a lower AF [= assessment factor] should be applied to the RAC derived from the most appropriate micro-/mesocosm study […] for the specific case, considering a weight of evidence approach. If the available micro-/mesocosm studies are of the same quality, the AF may be applied to the geometric mean value of the Effect class 1 or Effect class 2 concentrations derived from the different studies. " (EFSA, 2013, page 128).

Where a range is presented, EFSA (2013) gives some factors that can be considered for justification of a lower AF, apart from having more than one study:

- the number of replicates is higher than the minimum required to achieve acceptable MDDs;
- the number of exposure concentrations tested is larger than the minimum of five concentrations;
- a sufficient pre-treatment period has been included to allow the community to be well-established in the system. Nevertheless, a mesocosm study should always be pre-treated before the test;
- the ecological relevance and richness of species of the community tested is higher than expected for the situation to be assessed;
- more than the minimum 8 populations of sensitive/vulnerable taxa are present with acceptable MDD;
- the exposure concentrations tested are worst-case relative to the predicted exposure scenario (i.e. multiple peaks are tested where a single peak is predicted).

For the selection of an appropriate assessment factor to derive a $PNEC_{water}$ for biocides the proposal by Brock et al. (2011) is followed since this selection of the assessment factors is scientifically justified and was based on published data from mesocosm studies with substances of all indications (i.e. herbicides, fungicides and insecticides) mimicking short-term and chronic exposure, and is considered protective for continuous and non-continuous exposure.

The following assessment factors are proposed based on the discussions at the workshop:

Effect class 1: 2 - 4
Effect class 2: 4 - 5
Effect class 3A: If the recovery option is applicable (for criteria see 3.1.5), an assessment factor of at least 5 would be needed to derive a PNEC from a single Effect class 3A endpoint.

The height size of the assessment factor within the given range is based on expert judgment considering the quality of the study. If several mesocosm studies of comparable quality are available a lower assessment factor may be appropriate or the assessment factor can be based on the highest Effect class 1 or 2 for the environmental threshold option or Effect class 3A for the environmental recovery option. If the recovery option is not applicable, Effect class 3A concentrations may still be used as additional evidence to support Effect class 1 or 2 studies, or to underpin the assessment factor for an Effect Class 1 or 2 endpoints.

4. Summary

For the authorisation of biocides under Regulation 528/2012/EC the potential risk to the environment is assessed. In the instance, a base set consisting of laboratory studies reflecting worst-case conditions is considered. If risk is indicated, the assessment can be refined by refining the effect side using non-standard approaches (e.g. field data or model ecosystem studies). Besides some limitations (e.g. limited number or absence of long-living species as compared to field communities) model ecosystem studies (in this context referred to as mesocosm studies) are a valuable tool to study effects of chemicals with a greater environmental realism. In contrast to single species tests, mesocosm studies allow for the assessment of additional species interactions and secondary effects. Thus, endpoints reflect a higher level of biological organization. Information gathered from mesocosm studies can help to assess the impact on community structure and consequently, ensure long-term functioning of aquatic ecosystems. This guidance is seen as an extension of the TGD (2003) as it gives more and precise information and integrates current research and approaches used under other European legislation (2000/60/EC and 1107/2009/EC) thereby facilitation harmonization.

General guidance on the design of mesocosm studies is given by OECD (2006), EFSA (2013) and in various publications (e.g. CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999, ELINK edited by Brock et al. 2010a and de Jong et al. 2008). For biocides, special attention should be given to the anticipated exposure pattern in the field and whether recovery can be taken into account or not. An integrated understanding of the used endpoints will facilitate communication and will ease assessment of results. An overview is given which aligns the commonly used abbreviations (e.g. NOEAEC) to the respective Effect classes as described by de Jong et al. (2008).

A concept for the re-evaluation of mesocosm studies which were conducted for purposes other than the support of a biocidal registration authorisation (i.e. typically for plant protection products) is developed on the basis of different exposure patterns: single and multiple peak exposure. The re-evaluation scheme integrates scientific approaches developed and applied under other European legislation (e.g. 2000/60/EC). For studies with one single peak, dissipation time of the substance in water and the time to onset of effect are important criteria that are used to decide on the expression of the endpoint as nominal or time-weighted average value and the applicability of the study as $PNEC_{water}$. For the evaluation of studies with multiple peaks it has to be differentiated between two exposure patterns: (i) the substance

disappears between the peaks, (ii) the substance does not disappear completely. If the time span between peaks is longer than the standard laboratory study on the trophic level of interest and the onset of effects were visible before the next peak the mesocosm is evaluated as a single peak mesocosm experiment. If it is shorter, the focal point is whether the toxicity caused by continuous exposure is similar to toxicity caused by repeated exposure. Generally, a potential relevance of a study for the sediment risk assessment has to be kept in mind especially for substances that dissipate into sediment and are relatively stable (in) there.

In the TGD, 2003 the size of the assessment factor is left open. Based on current research and in relation to other European legislation it is proposed to set the assessment factor for a single mesocosm between 2 to 5. The exact size of the factor depends on the used Effect class, the applicability of recovery and the quality of the study. If more data (e.g. several mesocosm studies) are available a lower assessment factor may be applied.

5. References

Ashauer R, Wittmer I, Stamm C, Escher BI (2011). Environmental Risk Assessment of Fluctuating Diazinon Concentrations in an Urban and Agricultural Catchment Using Toxicokinetic–Toxicodynamic Modeling. Environmental Science & Technology, 45 (22), 9783-9792.

Beketov M.A., Schäfer R.B., Marwitz A., Paschke A., Liess M. (2008): Long-term stream invertebrate community alterations induced by the insecticide thiacloprid: Effect concentrations and recovery dynamics; Science of the total environment 405:96-108

Brock, T.C.M., Arts, G.H.P., Maltby, L., Van den Brink, P.J. (2006): Aquatic risks of pesticides, ecological protection goals, and common aims in European Union legislation; Integrated Environmental Assessment and Management 2(4): 20-46

Brock, T.C.M., Maltby, L., Hickey, C.W., Chapman, J., Solomon, K. (2008): Spatial extrapolation in ecological effect assessment of chemicals. In: Solomon et al. eds. Extrapolation practice for ecotoxicological effect characterization of chemicals, Chapter 7. Boca Raton, FL, USA: CRC Press (SETAC books).

Brock, T.C.M., Roessink, I., Belgers, J.D.M., Bransen, F. and Maund, S.J. (2009). Impact of a benzoyl urea insecticide on aquatic macro-invertebrates in ditch mesocosms with and without non-sprayed sections. Environmental Toxicology and Chemistry, 28, 2191–2205

Brock T.C.M., Alix, A., Brown, C., Capri, E., Gottesbüren, B., Heimbach, F., Lythogo C., Schulz, R., Streloke, M. (Eds.) (2010a): Linking aquatic exposure and effects. Risk assessment of pesticides. European Union Workshop on Linking Aquatic Exposure and Effects in the Registration Procedure of Plant Protection Products (ELINK). Bari, Italy and Wageningen, Netherlands, 2007. SETAC Press & CRC Press, Taylor & Francis group.

Brock T, Arts G, Belgers D and Van Rhenen-Kersten C, 2010b. Ecological characterization of drainage ditches in the Netherlands to evaluate pesticide stress. In: Linking aquatic exposure and effects: risk assessment of pesticides. Eds Brock TCM, Alix A, Brown CD, Capri E, Gottesbüren BFF, Heimbach F, Lythgo CM, Schulz R and Streloke M. SETAC Press & CRC Press, Taylor & Francis Group, Boca Raton, FL, USA, 269–287

Brock T.C.M., Arts, G.H.P., ten Hulscher, T.E.M., de Jong, F.M.W., Luttik, R., Roex, E.W.M., Smit, C.E., van Vliet, P.J.M. (2011): Aquatic effect assessment for plant protection products: A Dutch proposal that addresses the requirements of the plant protection Product regulation and Water Framework Direktive; Altera report

Campbell, P.J., Arnold D.J.S., Brock, T.C.M., Grandy, N.J., Heger, W., Heimbach, F., Maund, S.J., Streloke, M. (1999): Guidance document on higher-tier aquatic risk assessment for pesticides (HARAP), Setac-Europe, Brussels, 179p

De Jong, F.M.W., Brock, T.C.M., Foekema, E.M., Leeuwangh P. (2008): Guidance for summarizing and evaluating aquatic micro- and mesocosm studies; RIVM Report 601506009/2008Directive 2000/60/EC of the European parliament and of the council of 23 October 2000 establishing a framework for Community action in the field of water policy, Official Journal of the European Communities

EFSA (2013): ScientificScientificS opinion; Guidanceon tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters.

Giddings, J.M., Brock, T.C.M., Heger, W., Heimbach, F., Maund, S.J., Norman, S.M., Ratte, H.T., Schäfers, C., Streloke, M. (2002): Community-level aquatic system studies: interpretation criteria; Proceedings from the CLASSIC workshop; Setac, 60p

Klimisch H.J., Andreae, M., Tillmann, U. (1997): A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data; Regulatory Toxicology and Pharmacology, 25: 1-5

Liess, M. and Von der Ohe, P.C. (2005). Analysing effects of pesticides on invertebrate communities in streams. Environmental Toxicology and Chemistry, 24, 954–965.

Maltby L., Blake N., Brock T.C.M. and Van den Brink P.J. (2005): Insecticide species sensitivity distributions: the importance of test species selection and relevance to aquatic ecosystems. Environmental Toxicology and Chemistry, 24: 379-388

OECD (1998): Report of the OECD Workshop on Statistical Analysis of Aquatic Toxicity Data. Series on Testing and Assessment, No 10. OECD Environment Directorate, Paris

OECD (2001): Simulation Test - Aerobic Sewage Treatment: 303 A: Activated Sludge Units. OECD Environment Directorate, Paris

OECD (2006): Guidance document on Simulated Freshwater Lentic Field tests (outdor microcosms and mesocosms). Series on Testing and Assessment, No 53. OECD Environment Directorate, Paris

OECD (2006): Current approaches in the statistical analysis of ecotoxicity data: a guidance to application. Series on Testing and Assessment, No 54. OECD Environment Directorate, Paris

Regulation 1107/2009/EC (2009) concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC; Official Journal of the European Communities

Regulation 528/2012/EC of the European parliament and of the council of 22 May 2012 concerning the making available on the market and use of biocidal products; Official Journal of the European Communities

Sanco/3268/2001 rev.4 (2002): Guidance Document on Aquatic Ecotoxicology in the context of the Directive 91/414/EEC

Schmolke A., Thorbek P., DeAngelis D.L. & Grimm V. (2010): Ecological models supporting environmental decision making: a strategy for the future; Trends in Ecology & Evolution, 25: 479-486

Suter, G.W. and Cormier, S.M. (2011): Why and how to combine evidence in environmental assessments: weighing evidence and building cases; Science of Total Environment; 409:140-1417

TGD (2003): 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 product on the market; Part II, European Commission EUR 20418 EN/2

EC (2011): Common Implementation Strategy for the Water Framework Directive (2000/60/EC). Guidance Document No. 27. Technical Guidance For Deriving Environmental Quality Standards. Brussels, Belgium. European Commission. Technical Report - 2011 - 055

Van den Brink, P.J., Van Wijngaarden, R,P,A,, Lucassen, W,G,H,, Brock, T,C,M, and Leeuwangh, P, (1996). Effects of the insecticide Durban 4®E (a.i. chlorpyrifos) in outdoor experimental ditches: II. Community responses and recovery. Environmental Toxicology and Chemistry, 15, 1143–1153.

Von der Ohe P.C., Dulio V., Slobodnik J., De deckere E., Kühne R., Ebert R.U., Ginebreda A., De Cooman W., Schüürmann G. and Brack W. (2011): A new risk assessment approach for the prioritization of 500 classical and emerging microcontaminants as potential river basin specific pollutants under the European water Framework Directive; Science of the total Environment; 409: 2064-2077

Table 8-4: Overview of emission patterns per product-type

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
Main group 1: Disinfectants						
PT 1	Human hygiene	EUBEES RIVM/Haskoning 2004	Private use (based on tonnage or on average consumption)	waste water	N	
			Skin and hand application in hospitals (based on tonnage or on average consumption)	waste water	N	
PT2	Disinfectants and algaecides not intended for direct application to humans or animals	JRC 2011	Industrial and institutional areas	waste water	N	
			Air conditioning	waste water	N	
			Hospital waste			
			Chemical toilets	waste water	N	
		RIVM 2001	Sanitary sector (based on tonnage or on average consumption	waste water	N	
			Room, furniture and objects in the medical sector	waste water	N	
			Instruments in medical sector (endoscopes)	waste water	N/Y	potentially not continuous in case of large replacement interval
			Instruments in medical sector (other instruments)	waste water	N	
			Laundry disinfection	waste water	N	
		OECD 2004/RIVM 2002	Swimming pools	waste water, water	N/Y	potentially not continous in case of draining private pools; relevance not fully clear
PT3	Veterinary hygiene	JRC 2011	Disinfection of animal housings	slurry	Y	in case of higher tier modelling
			Disinfection of vehicles	waste water	N	
			Teat dips	slurry	Y	id.
			Footwear/animals feet	slurry	Y	id.

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
			Hatcheries	waste water	N	
PT4	Food and feed area	JRC 2011	Food, drink and milk industry	waste water	N	
			Large scale catering kitchens, canteens., slaughterhouses, etc.	waste water	N	
			Milking parlour systems	waste water	N	
PT5	Drinking water	EUBEES/UBA 2003	Disinfection in distribution system	waste water	N	
Main group 2: Preservatives						
PT6	Preservatives for products during storage	EUBEES RIVM/Haskoning 2004	In-can preservatives; ESD refers to PT8 and 21 for direct emissions to water	waste water, water	N	application phase not continuous, but service life is main driver for risk assessment = continuous
		EUBEES Ineris 2001	Paper coating and finishing PT6, 7 and 9	waste water	N	
PT7	Film preservatives	EUBEES RIVM/Haskoning 2004	Paints and coatings: refers to PT8 for direct emissions to water	waste water, water	N	
		EUBEES Ineris 2001	Paper coating and finishing PT6, 7 and 9	waste water	N	
PT8	Wood preservatives	OECD 2012	industrial use (impregnation and surface treatment) / application	waste water	N	
			industrial use (impregnation and surface treatment) / storage	water via runoff	N	
			in situ application : bridge over pond	water	N	application phase not continuous, but service life is main driver for risk assessment = continuous
			use class 3,1 - external, no ground contact / house	not relevant		
			use class 3,1 - external, no ground contact / noise barrier	waste water	N	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
			use class 3,1 - external, no ground contact / bridge over pond	water	N	
			use class 4,1 - external, with ground contact, permanently	not relevant		
			use class 4,2 - external, with water contact, permanently	water	N	
			use class - in seawater, permanently	water	N	
PT9	Fibre, leather, rubber and polymerised materials preservatives	EUBEES Ineris 2001	Leather tanning	waste water	N	
		EUBEES Ineris 2001	Textile processing	waste water	N	
		EUBEES RIVM/Haskoning 2004	Rubber and polimerised materials			
			Rubber	waste water, water	N	
			Plastic	waste water, water	N	
			Textile	waste water, water	Y/N	direct emissions from treated textile to water?
		EUBEES Ineris 2001	Paper coating and finishing PT6, 7 and 9	waste water	N	
PT10	Construction material preservatives	EUBEES Ineris 2002	In-situ treatment (currative) in the city	waste water, water	N	application phase not continuous, but service life is main driver for risk assessment = continuous
			Preservative treatment (in-situ or elsewhere) in the city	waste water, water	N	
PT11	Preservatives for liquid-cooling and processing systems	EUBEES RIVM 2003	Once-through, shock/continuous	water	Y	Only for shock treatment
			Open-recirculating, shcock/continuous	waste water, water	N	
			Closed, shock/continuous	waste water, water	N	
PT12	Slimicides	EUBEES RIVM/Haskonin	Paper mill	waste water	N	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
		g 2003	Offshore oil exploitation (reservoir injection, oil storage systems, etc.)	seawater	N	
			Offshore oil exploitation (workover chemicals, closed drain systems, etc)	seawater	Y	
PT13	Working or cutting fluid preservatives	EUBEES RIVM/Haskoning 2003	Metal working machines	waste water	N	
Main group 3: Pest control						
PT 14	Rodenticides	EUBEES DK EPA 2003	Sewer systems	waste water	N	
			In and around buildings	waste water	N	
PT 15	Avicides	EUBEES 2003	Bait preparation	waste water	N	
			In and around buildings	waste water	N	
PT 16	Molluscicides, vermicides and products to control other invertebrates	No ESD				
PT 17	Piscicides	No ESD				
PT 18	Insecticides, acaricides and products to control other arthropods	OECD 2006	Animal housings and manure storage	waste water, slurry, manure	Y	in case of higher tier modelling
		EUBEES Ineris 2001	Textile processing	waste water	N	
		OECD 2008	Insecticides, acaricides, control arthropods			
			Indoor applications	waste water	N	
			Outdoor applications (urban), rain water	waste water, water	N	
			Outdoor applications rural	not relevant		
			Outdoor application, vector control	water	Y	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
			Outdoor application near water pond (biocidal treatment on trees)	water (via drift)	Y	
PT 19	Repellents and attractants	No ESD				
PT 20	Control of other vertebrates	No ESD				
Main group 4: Other biocidal products						
PT 21	Antifouling products	EC 2004	Marina, commercial harbour, shipping lane	water	N	
PT 22	Embalming and taxidermist fluids	EUBEES Ineris 2001	Taxidermy, embalming	waste water	N	

Appendix 9 – Additional guidance from other legislations

In case the guidance provided in this Volume is not sufficient to cover the exposure, effect or risk assessment for a biocidal active substance, e.g. in case of very specific uses or substance properties, the following guidance documents from other legislations could be used as advisory documents:

1. if the chemical is difficult, which implies amongst others hydrophobic, extra guidance is given in OECD aquatic toxicity and difficult substances and mixtures
2. for mixtures, use OECD aquatic toxicity and difficult substances and mixtures
3. Guidance developed within the context of Regulation (EC) No 1907/2006 (REACH)
4. Guidance developed within the context of Directive 91/414/EEC i.e.:
   General guidance for ecotoxicity:
   a. Guidance Document on Aquatic Ecotoxicology under Council Directive 91/414/EEC -
   b. Guidance Document on Terrestrial Ecotoxicology Under Council Directive 91/414/EEC -

   Groundwater modelling guidance documents:
   - FOCUS groundwater scenarios in the EU review of active substances
   - Generic guidance for FOCUS groundwater scenarios

   Assessment of degradation studies
   - Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration

   Risk assessment
   - European Guidance Document on Risk Assessment for Birds and Mammals – working document
   - EPPO Standards - Environmental risk assessment scheme for plant protection products
     Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters (EFSA Journal 2013; 11(7):3290)

EUROPEAN CHEMICALS AGENCY
ANNANKATU 18, P.O. BOX 400,
FI-00121 HELSINKI, FINLAND
ECHA.EUROPA.EU