TECHNICAL GUIDANCE DOCUMENT IN SUPPORT OF 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

PART II

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TECHNICAL GUIDANCE DOCUMENT IN SUPPORT OF

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

Part II

Document

FOREWORD

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THE COMMISSION DIRECTIVE 93/67/EEC ON RISK ASSESSMENT FOR NEW NOTIFIED SUBSTANCES AND THE COMMISSION REGULATION (EC) 1488/94 ON RISK ASSESSMENT FOR EXISTING SUBSTANCES

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Chapter 3

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1. General introduction

1.1 Background

Commission Directive 93/67/EEC and Commission Regulation (EC) No. 1488/94 require that an environmental risk assessment be carried out on notified new substances or on priority existing substances, respectively. This risk assessment should proceed in the following sequence:

- Hazard identification;
- Dose (concentration) - response (effect) assessment;
- Exposure assessment;
- Risk characterisation.

The risk assessment shall be carried out for all three environmental compartments, i.e. aquatic environment, terrestrial environment and air.
The present document is intended to assist the competent authorities to carry out the environmental risk assessment of notified new substances and priority existing substances. This guidance document includes advice on the following issues:

- how to calculate PECs and PNECs (sections 2 and 3, respectively) and, where this is not possible, how to make qualitative estimates of environmental concentrations and effect/no effect concentrations;
- how to judge which of the possible administrative decisions on the risk assessment according to Article 3(4) of Directive 93/67/EEC or Article 10 of Regulation 793/93 and Annex V of Regulation 1488/94 need to be taken (section 4);
- how to decide on the testing strategy, if further tests need to be carried out and how the results of such tests can be used to revise the PEC and/or the PNEC (section 5).

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

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

The risk assessment should be carried out on the basis of all data available applying the methods described in the following sections of the document.

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

The guidance has been developed mainly from the experience gained on individual organic substances. This implies that the risk assessment procedures described cannot always be applied without modifications to specific 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 special appendices to this guidance document (Appendix VIII, IX and XI respectively). In these appendices, it is indicated as much as possible where the text of the main document applies and where not. Where necessary, specific methods are described.

The risk assessments that have to be carried out according to Regulations 793/93 and 1488/94 for existing substances and Directives 67/548/EEC and 93/67/EEC for new substances, respectively, are in principle valid for all countries in the European Union. It is recognised however, that especially the exposure situation in different countries can vary extremely e.g. due to topographical and climatological differences. Therefore in this document in the first stage of the exposure assessment where exposure models are used, so-called generic exposure scenarios are applied.

This means that it is assumed 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 or to sea water are not assessed. Neither are site specific assessments drawn up. When more specific information on the emission scenario 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 only be carried out qualitatively because no adequate biotic testing systems are available. 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 reviewed and, if necessary, revised when further scientific knowledge and experience becomes available.

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

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

Some of these effects may occur with substances that are persistent under environmental conditions and that tend to bioaccumulate. Therefore, it is advisable to take special care in the risk assessment procedure of such substances.

In the current document, the risk assessment for the aquatic ecosystem basically deals with the freshwater systems only. So far, the experience is not sufficient to give practical guidance for the assessment of marine ecosystems, as regards characteristics such as the extremely large dilution, low biodegradation rates, long-term exposure and effects on saltwater organisms.

Furthermore 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 4.5).

1.2 General principles of assessing environmental risks

In essence, the procedure for the environmental risk assessment of a substance consists of comparing the concentration in the environmental compartments (predicted environmental concentration (PEC)) with the concentration below which unacceptable effects on organisms will most likely not occur (predicted no effect concentration (PNEC)). In principle, human beings as well as ecosystems in the aquatic, terrestrial or air compartment are to be protected. For the environment the protection goals at present are limited to the following:

- Aquatic ecosystem;
- Terrestrial ecosystem;
- Top predators;
- Micro-organisms in sewage treatment systems;
- Atmosphere.

In addition to the three primary environmental compartments, effects not specific to a particular compartment which are relevant to the food chain (secondary poisoning) are considered as well as effects on the microbiological activity of sewage treatment systems. The latter is evaluated because proper functioning of waste water treatment plants (STPs) is important for the exposure of the aquatic environment.
The PECs can be derived from available monitoring data and/or model calculations. The PNEC values are usually determined on the basis of results from monospecies laboratory tests or, in a few cases established concentrations from model ecosystem tests, taking into account adequate safety factors. A PNEC is regarded as a concentration below which an unacceptable effect will most likely not occur.
Dependent on the PEC/PNEC ratio the decision whether a substance presents a risk to organisms in the environment is taken. If it is not possible to conduct a quantitative risk assessment, either because the PEC or the PNEC or both cannot be derived, a qualitative evaluation is carried out of the likelihood that an adverse effect may occur.
As will be explained in more detail in the section on exposure assessment, PEC values are derived for local as well as regional situations, each of them based on a number of specific emission characteristics with respect to time and scale. As a consequence, a combination of PNEC values for the different compartments/protection goals with different PEC values (or exposure concentrations for microbiological activity for STP) for different exposure scenarios can lead to a number of PEC/PNEC ratios.

Table 1 shows a summary of the different endpoints of the risk characterisation and the exposure scenarios to which they apply. In addition to the PECs mentioned in Table 1, several other exposure levels are derived in section 2. These are used for the assessment of indirect human exposure through the environment, which is described in the Technical Guidance Document on Risk Assessment for Human Health (Chapter 2). The PECs that are specifically derived for this indirect exposure assessment are summarised in Table 2.

Table 1 *Relationship between different endpoints in the risk characterisation for different exposure media*

Target	**Medium of exposure (PEC_{local} / $PEC_{regional}$)**	**section**	**PNEC**	**section**
Aquatic organisms	surface water	2.3.8.3 & 2.3.8.7	$PNEC_{water}$	3.3
Benthic organisms	sediment	2.3.8.4 & 2.3.8.7	$PNEC_{sed}$	3.5
Terrestrial organisms	agricultural soil	2.3.8.5 & 2.3.8.7	$PNEC_{soil}$	3.6
Fish eating predators	fish	3.8	$PNEC_{oral}$ from $NOAEL_{avian/mammalian}$	3.8
Worm eating predators	earthworms	3.8	$PNEC_{oral}$ from $NOAEL_{avian/mammalian}$	3.8
Micro-organisms	STP aeration tank	2.3.7	$PNEC_{micro-organisms}$	3.4

Table 2 *Exposure levels used for indirect human exposure*

Target	**Medium of exposure (PEC_{local} / $PEC_{regional}$)**	**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 over 180 days)	2.3.8.5 & 2.3.8.7
Fish for human consumption	Surface water (annual average)	2.3.8.3 & 2.3.8.7

2. Environmental exposure assessment

2.1 Introduction

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

- Production;
- Processing;
- Transport and storage;
- Formulation (blending and mixing of substances in preparations);
- Use:
  - Professional large scale use (industry) and/or;
  - Professional small scale use (trade) and/or;
  - Private or consumer use;
- Disposal, including waste treatment (e.g. incineration and recycling).

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

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

Consideration should be given to whether the substance being assessed can be degraded, biotically or abiotically, to give stable and/or toxic degradation products. Where such degradation can occur, the assessment should give due consideration to the effects which might arise. For new substances, it is unlikely that information will be available on such degradation products and thus only a qualitative assessment can be made. For HPV substances, however, known significant degradation products should also be subject to risk assessment. Where no information is available, a qualitative description of the degradation pathways can be made. A summary of some of these is presented in Appendix X.

In many situations available biodegradation data is restricted to aerobic conditions, however, in some situations, e.g. sediment or ground water, anaerobic conditions should also be considered.
Salinity and pH are examples of other environmental conditions that may influence the degradation.

2.1.1 Measured / calculated environmental concentrations

For new substances, usually no relevant measured data will be known. Therefore, concentrations of a substance in the environment must be estimated. Unlike for new substances, the exposure assessment of existing substances does not always depend upon modelling. Data on measured levels in various environmental compartments have been gathered for a number of substances. They can provide the potential for greater insight into specific steps of the exposure assessment procedure (e.g. concentration in industrial outfalls, "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 manufacturing and use of the substance, or may be due to assumptions in or limitations of the modelling or measurement procedures. It may seem that measurements always give more reliable results than model estimations. However, measured concentrations can have a considerable uncertainty associated with them, due to temporal and spatial variations. Both approaches complement each other in the complex interpretation and integration of the data. Therefore the availability of adequate measured data does not imply that PEC calculations are unnecessary.

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

2.1.2 Relation between PEC_{local} and $PEC_{regional}$

For the release estimation of substances, a difference 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 have a major impact on the environmental concentration on a local scale (PEC_{local}) and contribute to the environmental concentrations on a larger scale ($PEC_{regional}$).

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

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

$PEC_{regional}$
The 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.

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

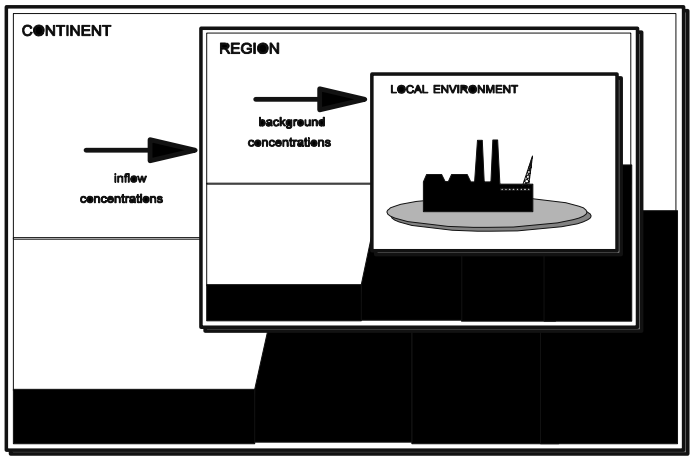

Figure 1 *The relations between the continental, regional, and local scale exposure assessments*

This implies that the continental, regional, and local calculations must be done sequentially. It should be noted that the use of regional data as background for the local situation may not always be appropriate. In the extreme case that 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 also is responsible for the background concentration of the region.

2.2 Monitoring data

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

The following stepwise procedure should be followed in the evaluation:

- Reliable and representative data have to be selected by evaluation of the sampling and analytical methods employed and the geographic and time scales of the measurement campaigns (section 2.2.1).
- The data have to be assigned to local or regional scenarios by taking into account the sources of exposure and the environmental fate of the substance (section 2.2.2).
- The monitoring data should be compared to the corresponding calculated PEC. For risk characterisation, a choice should be made between using monitoring data or a calculated PEC (section 2.5).

2.2.1 Selection of adequate monitoring data

Firstly, the available measured environmental concentrations have to be verified. To be able to decide if the data are adequate for use in the exposure assessment and how much importance should be attached to them, the following aspects must be considered:

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

The detection limit of the analytical method 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 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.

Selection of representative data for the environmental compartment of concern
It has to be ascertained if the data are results of sporadic examinations or if the chemical was detected at the same site over a certain period of time. Measured concentrations caused by an accidental spillage or malfunction should not be considered in the exposure assessment. Data from a prolonged monitoring program, where seasonal fluctuations are already included, are of special interest. If available, the 90-percentile values of the measured data are of highest preference. If only maximum concentrations are reported, they should be considered as a worst-case assumption, whereas using the average concentrations can result in an underestimation of the existing risk, because temporal and/or spatial average concentrations do not reflect periods and/or locations of high exposure.

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

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

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

Evaluation of the geographical relation between emission sources and sampling site

If there is no spatial proximity between the sampling site and point sources of emission (e.g. from rural regions), the data represent a background 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, (e.g. data from a monitoring program in an industrial area), they are of a PEC_{local}-type. In a PEC_{local} based on measured concentrations, the background concentration is already included.

Consideration of specific properties of the substance

Based on the physico-chemical properties of a substance, its behaviour in the different environmental compartments has to be considered for the evaluation of monitoring data.

2.3 Model calculations

2.3.1 Introduction

The first step in the calculation of the PEC is evaluation of the primary data. The subsequent step is to estimate the substance's release rate based upon its use pattern. All potential emission sources need to be analysed, and the releases and the receiving environmental compartment(s) identified. After assessing releases, the fate of the substance once released to the environment needs to be considered. This is estimated by considering likely routes of exposure and biotic and abiotic transformation processes. Furthermore, secondary data (e.g. partitioning 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_{local} and $PEC_{regional}$. The PEC calculation is not restricted to the primary compartments; surface water (section 2.3.8.3), soil (section 2.3.8.5) and air (section 2.3.8.2); but also includes secondary compartments such as sediments (section 2.3.8.4) and groundwater (section 2.3.8.6). Transport of the substance between the compartments must, where possible, be taken into account.

This section is organised as follows:

- Description of the minimal data set requirements for the distribution models described in the following sections;
- Estimation of releases to the environment;
- Definition of the characteristics of the standard environment used in the estimation of PECs on the local and regional scale;
- Derivation of secondary data: intermedia partitioning 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 (local and regional).

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

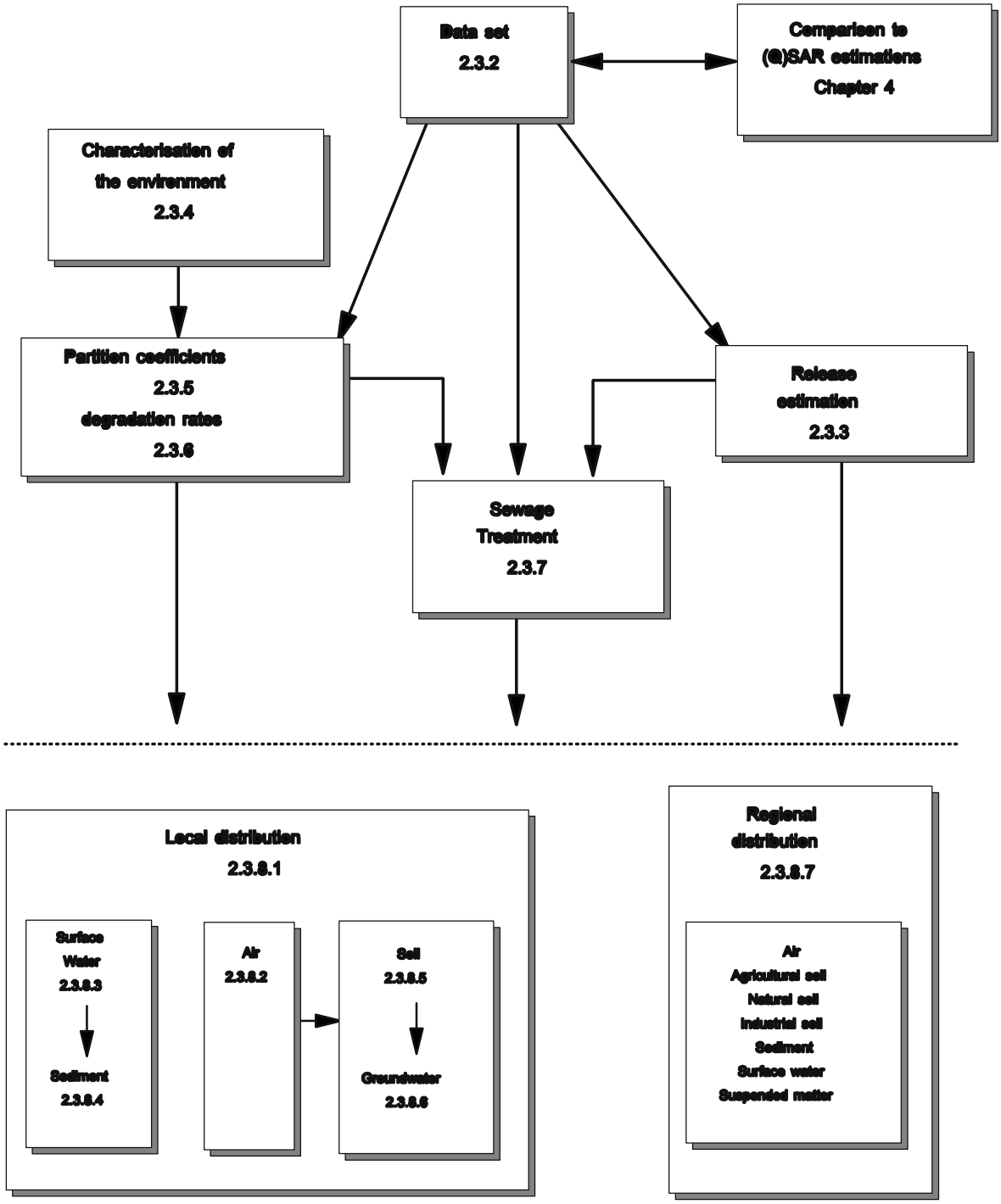

Figure 2 *Organisation of section 2.3, including the flow of data between the different sections*

In each section, the model calculations are given. For the explanation of symbols used in an equation, the following table format is used:

Explanation of symbols:

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

For the symbols, as much as possible, the following conventions will be applied:

- 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 generally occurring symbols are:

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 chemical	[$mg.kg^{-1}$] 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 Foc_{soil} means the fraction (*F*) organic carbon (*oc*) in the soil compartment ($_{soil}$). For other parameters, interpretable symbols are chosen. It should be noted that in several equations fixed factors (e.g. 1000 or 10^6) are applied. This is done to make the equations consistent with regard to the units of parameters.

2.3.2 Data for exposure models

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

Physico-chemical properties:

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

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

Use pattern of the substance:

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

In section 2.3.5 and 2.3.6, it is described how secondary data (partition coefficients and degradation rates) are derived from the minimally required data. 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. For other types of substances, more specific information (e.g. partitioning coefficients or pKa/pKb for ionising substances) may be required. For ionising substances, the pH-dependence of Kow and water solubility should be known. Partitioning coefficients should preferably be corrected according to the pH of the environment (see Appendix XI).

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

If experimentally determined physico-chemical data have been obtained at a temperature which for the substance under consideration significantly would change when extrapolated to the relevant temperature of the employed exposure models (e.g. 13 ^{o}C in the regional model) then such an extrapolation should be considered. In most cases this will not be necessary. The vapour pressure, however may for some substances change considerably according to the temperature even within a temperature range of only 10 ^{o}C. in such cases an estimated vapour pressure at the relevant temperature should be obtained either by interpolation from the vapour pressure at 10 ^{o}C and 20 ^{o}C or by use of extrapolation methods (Schwartzenbach et al., 1993).

2.3.3 Release estimation

In this section, the following parameters are derived:
- local emission rates to air and wastewater during an emission episode
- regional emissions to air, wastewater, and industrial soil (annual averages)

2.3.3.1 Life cycle of substances

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

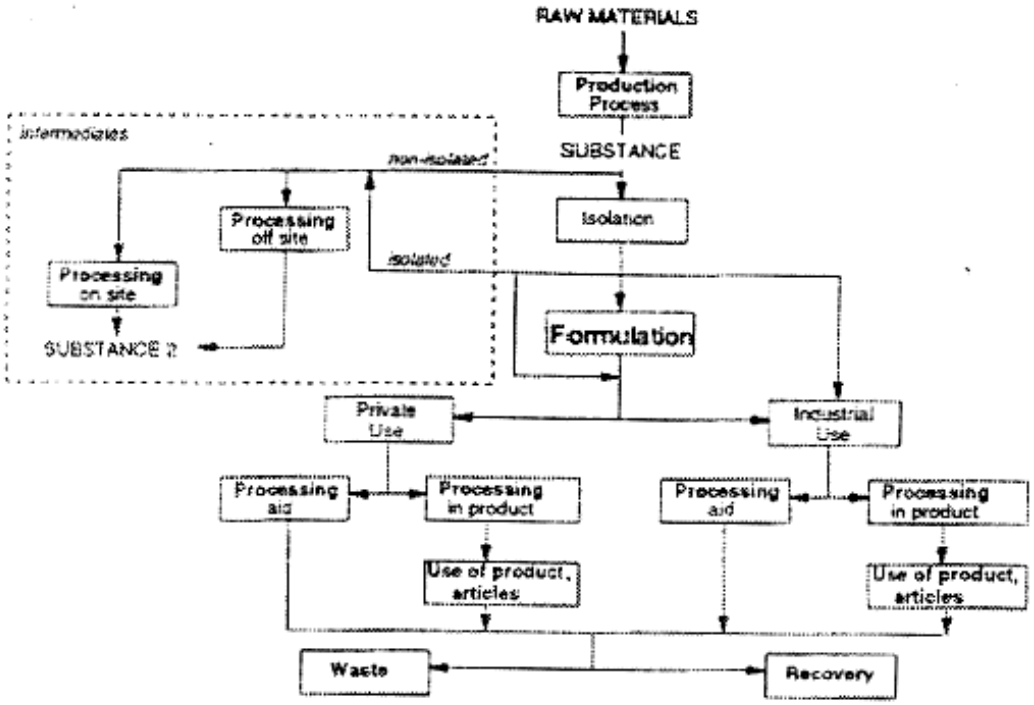

Figure 3 *Schematic representation of the life cycle of a substance*

Production

Production is the stage where the substance is manufactured, i.e. formed by chemical reaction(s), isolated, purified, drummed or bagged, etc. For intermediates (chemicals used to make other chemicals) a distinction is made between non-isolated intermediates, site-limited, and captive and other intermediates, as can be seen in Figure 3. "Non-isolated" means that the substance is not isolated from the reaction mixture but transformed directly into another substance in the same equipment in a subsequent reaction step. "Site-limited" means that the substance is manufactured and consumed at the same site.

This signifies that releases at production and processing (the transformation into the next substance) occur at the same site. "Captive" means that the intermediate is manufactured and shipped to other sites owned by the same company, but not sold to others. Therefore, releases at production of captive and other intermediates occur at another site as where the substance is transformed into the next substance.

Formulation

Formulation is the stage where chemicals are combined in a process of blending and mixing to obtain a product or preparation. This may be a formulation like a paint, or a product like a photographic film. Formulations are applied or used at the next stage of the life-cycle (processing).

Processing

The stage of processing consists of all kinds of processes where the substance as such, a formulation, or an article containing the substance assessed, is applied or used. Substances may be used as a processing aid or be incorporated in a product. An example of a processing aid is a developer used in a photographic bath which is disposed of after use. It should be noted that the manufacture of photographic film and paper might also be considered as processing of the chemicals involved. However, these materials will be processed again after exposure (developing and fixing). So, manufacture of photographic films and paper is considered as the stage of formulation. Articles like a plastic toy or articles with a coating layer containing the substance assessed will be used during a certain range of years. Releases into the environment during this period due to migration, leaching and evaporation will increase to a maximum after the introduction of the substance, and subsequently decrease. Processing can take place at a very large scale at one or only a few sites in industry or at a professional small scale.

Private use

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

Disposal

At the stage of disposal, the substance (or the products containing the substance) is disposed of with waste or waste water. Waste treatment may exist of incineration and dumping. Release at these processes have not been taken into account so far, as there are no or insufficient data on leaching from landfills and escape of non-degraded substances at incineration. At this stage also recovery processes may occur. At recovery, two different situations have to be considered. Firstly, the substance assessed may be recovered and recycled. In this case releases will be limited. Secondly, another substance or product may be recycled, and the substance assessed is present in this product. Releases in this situation will be much higher as a rule, as the attention is not focused on the substance assessed, but on the substance or product recovered.

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

2.3.3.2 Types of emissions and sources

Emission patterns vary widely from well defined point sources (single or multiple) to diffuse releases from large numbers of small point sources (like households) or line sources (like a motorway with traffic emissions), and from continuous to intermittent releases. Continuous emissions are characterised by an almost constant emission rate flow over a prolonged period (e.g. the emission of a substance from a continuous production process such as an oil refinery). Intermittent emissions can be peak emissions or block emissions (see section 2.3.4.4). Peak emissions are characterised by a relatively large amount discharged in a short time where the time intervals between peaks and the peak height can vary greatly (e.g. the discharge of spent liquid - reaction mixture - after isolation of the synthesised substance in a batch process). Block emissions are characterised by a flow rate which is reasonably constant over certain time periods with regular intervals with a low or even zero background emission (e.g. the emissions from traffic during the day; during rush hours emission are high in particular). The quantities released at a certain process may vary from 100%, as is the case for example with household products like detergents or volatile solvents in paints, to below 1% for substances like intermediates produced in closed systems.

2.3.3.3 Release estimation

It is clear that the releases of a substance are dependent on the use patterns. Three types of categories are distinguished, i.e. main category, industrial category and function or use category. An overview of these categories can be found in Chapter 5. The main categories are intended to describe generally the exposure relevance of the use(s) of a substance. In the context of environmental risk assessment they are also used to characterise release scenarios for the estimation of emissions to the environment during specific stages of the life cycle of the substance (production, formulation, and processing). They can therefore be allocated to release fractions which are used as default values where specific information is missing. "Use in closed systems" as such, refers to the processing stage when a substance is used in a transformer or a circulation circuit of refrigerator; on the other hand it may refer to the stage of production where a substance like an intermediate is manufactured in closed apparatus. "Use resulting in inclusion into or onto a matrix" may refer 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 substance applied as a uv-stabiliser in paint ends up in the finished coating layer.

"Non-dispersive use" and "wide dispersive use" are related to the number (and size) of the emission sources.

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

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

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

It should be noted that considerable emissions may occur at another category than the one where a substance has been allocated to. A substance used in a paint will 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.

An example is the application of an additive for an epoxy resin applied in the electronic industry for the embedding of electronic components. Though the processing takes place at category 4 "Electrical/electronic engineering industry" the processing of epoxy resins belongs to category 11 "Polymers industry". The releases of the process will be found in the table for the latter category.

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. Chemicals 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 type of application are e.g. adhesives, cosmetics, detergents, and pharmaceuticals. Some applications have been covered in other industrial categories at the stage of private use. These applications comprise fuels and fuel additives (mineral oil and fuel industry), paint products (paints, lacquers and varnishes industry) and photochemicals (photographic industry). For industrial category 6 (public domain), use and application at public buildings, streets, parks, offices, etc. is considered.

The A-tables of Appendix I provide the estimated total release fractions of the production volume (emission factors) to air, (waste) water and industrial soil during production, formulation, processing, private use, and recovery, according to their industrial category. The production volume is defined as the total tonnage of a substances 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 volumes exported from the EU excluding the volumes 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 I 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. Further details are included in Appendix I. The estimations for new substances tend to be more conservative as less information is available than for existing substances. However, any relevant information provided by industry can be used to override the default values of the release tables.

To obtain the best entry to the tables for emission factors, Appendix I also contains a list of synonyms for functions of substances. The synonyms and their definitions have been derived from the US-EPA ChemUSES list (US-EPA, 1980).
In general, the data supplied by industry will help to find the correct entry to the release tables apart from the classification specified in Chapter 5.

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

$$TONNAGE = PRODVOL + IMPORT - EXPORT \quad (1)$$

Explanation of symbols

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

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

i	stage of the life cycle	*j*	compartment
1	production	a	air
2	formulation	w	water
3	processing	s	industrial soil (regional only)
4	private use		
5	recovery		

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

Input

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

Output

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

For each stage, the losses in the previous stage are taken into account (see calculation in Appendix I). Note that releases during production are not taken into account in the other stages, as generally, these releases will already be accounted for in the reported production volume. In certain cases this might lead to total releases exceeding 100%. The rapporteur must specify if releases during each phase are relevant or not. If the release during a certain life stage is not applicable, the release fraction will be set to zero.

After losses during the five stages of the life-cycle are accounted for, 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 not available. Furthermore, no quantitative methods have for example been developed for estimation of the emissions during the life of articles containing the substance regarded (main category II) e.g. a flame retardant in plastics used for tv-sets, radios etc.. However, even though quantitative methodologies are presently lacking for these types of emissions, preliminary quantitative estimations may be performed case-by-case.

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:

$$Elocal_{i,j} = Fmainsource_i \bullet \frac{1000}{Temission_i} \bullet RELEASE_{i,j} \quad (2)$$

Explanation of symbols:

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

For local release estimates, point sources (and therefore, presumably single stages of the life cycle) need to be identified. It will normally be necessary to assess each stage of the life-cycle to determine whether adverse effects can occur since decisions need to be made to clarify or reduce any identified risk for all life-cycle stages. This is not required if it is obvious that a certain stage is negligible. For the regional scale assessments, the release fractions for each stage of the life cycle need to be summed for each compartment. The emissions are assumed to be a constant and continuous flux during the year. Regional emissions can be calculated as:

$$Eregional_j = \frac{1000}{365} \bullet \sum_{i=1}^{5} RELEASE_{i,j} \quad (3)$$

Explanation of symbols:

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

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

- Especially HPV substances 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} shall be calculated by summing all the relevant emissions from that location. For releases to waste water, 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, emissions during this time will increase (e.g. a plastic article or a paint coating where the substance assessed is applied as a plasticiser).
  More guidance on this point needs attention in near future;
- Emission reduction techniques have not been taken into account in the tables of Appendix IA as the kind of techniques applied (with possibly large differences in efficiencies) as well as the degree of penetration may differ between Member States or industry sectors. Only when for a certain process a specific reduction measure is common practice this will be taken into account. In all other cases, reasonable worst-case applies.

2.3.3.4 Intermittent releases

Many substances are released to the environment from industrial sources as a result of batch, rather than continuous, processes. In extreme cases, substances may only be emitted a few times a year. Since the PECs associated with industrial releases can take into account both the amount released and the number of days of emission, the magnitude of the PECs in the risk assessment should not be affected. PEC_{local} 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, $PEC_{regional}$ is calculated using the annual release rate. It represents the steady-state concentration to be expected, regardless of when the discharge occurred.

Intermittent release needs to be defined, although rapporteurs will have to justify the use of this scenario on a case-by-case basis. Intermittent release can be defined as:

- intermittent but only recurring infrequently i.e. less than once per month and for no more than 24 hours.

This would correspond to a typical batch process only required for a short period of the year (releases to the environment may be only of limited duration). Thus, for the aquatic compartment, transport processes may ensure that the exposure of aquatic organisms is of short duration. Calculation of the likely exposure period should take into account the potential of a substance to substantially partition to the sediment. Such partitioning, while reducing the calculated $PEClocal_{water}$ may also increase the exposure time by repartitioning to the water phase over an extended period. For intermittent releases to the aquatic compartment a dedicated PNEC is used in the risk characterisation (see section 3.2.2).

Where the batch process occurs more frequently than above or is for a longer duration, protection from 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.

2.3.4 Characterisation of the environmental compartments

In this section, the following parameters are derived:
- definition of the standard environmental characteristics (Table 3)
- bulk densities for soil, sediment, and suspended matter

For the derivation of PECs at the local and regional scale, one standardised generic environment needs to be defined since we are aiming for one risk characterisation at EU level. The characteristics of the real environment will, obviously, vary in time and space. In Table 3, average or typical default values are given for the parameters characterising the environmental compartments (the values are chosen equal on both spatial scales). The standard assessment needs to be performed with the defaults, as given in Table 3. 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 3.

Several other generic environmental characteristics, mainly relevant for the derivation of $PEC_{regional}$ (e.g. the sizes of the environmental compartments, mass transfer coefficients) are given in section 2.3.8.7 (Table 10, Table 11, and Table 12).

Table 3 *Definition of the standard environmental characteristics*

Parameter	Symbol	Unit	Value
General			
Density of the solid phase	RHOsolid	[$kg_{solid}.m_{solid}^{-3}$]	2500
Density of the water phase	RHOwater	[$kg_{water}.m_{water}^{-3}$]	1000
Density of air	RHOair	[$kg_{air}.m_{air}^{-3}$]	1.3
Temperature (12°C)	TEMP	[K]	285
Surface water			
Concentration of suspended matter (dry weight)	$SUSP_{water}$	[$mg_{solid}.l_{water}^{-1}$]	15
Suspended matter			
Volume fraction solids in susp. matter	$Fsolid_{susp}$	[$m_{solid}^{3}.m_{susp}^{-3}$]	0.1
Volume fraction water in susp. matter	$Fwater_{susp}$	[$m_{water}^{3}.m_{susp}^{-3}$]	0.9
Weight fraction organic carbon in susp. solids	Foc_{susp}	[$kg_{oc}.kg_{solid}^{-1}$]	0.1
Sediment			
Volume fraction solids in sediment	$Fsolid_{sed}$	[$m_{solid}^{3}.m_{sed}^{-3}$]	0.2
Volume fraction water in sediment	$Fwater_{sed}$	[$m_{water}^{3}.m_{sed}^{-3}$]	0.8
Weight fraction organic carbon sediment solids	Foc_{sed}	[$kg_{oc}.kg_{solid}^{-1}$]	0.05
Soil			
Volume fraction solids in soil	$Fsolid_{soil}$	[$m_{solid}^{3}.m_{soil}^{-3}$]	0.6
Volume fraction water in soil	$Fwater_{soil}$	[$m_{water}^{3}.m_{soil}^{-3}$]	0.2
Volume fraction air in soil	$Fair_{soil}$	[$m_{air}^{3}.m_{soil}^{-3}$]	0.2
Weight fraction organic carbon in soil solids	Foc_{soil}	[$kg_{oc}.kg_{solid}^{-1}$]	0.02
Weight fraction organic matter in soil solids	Fom_{soil}	[$kg_{om}.kg_{solid}^{-1}$]	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 independent 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:

$$RHO_{comp} = Fsolid_{comp} \cdot RHOsolid + Fwater_{comp} \cdot RHOwater + Fair_{comp} \cdot RHOair \quad \text{with } comp \in \{soil, sed, susp\} \tag{4}$$

Explanation of symbols:

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

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

Total bulk density of the environmental compartments:

RHO_{susp}	Bulk density of (wet) suspended matter	[$kg.m^{-3}$]	1150
RHO_{sed}	Bulk density of (wet) sediment	[$kg.m^{-3}$]	1300
RHO_{soil}	Bulk density of (wet) soil	[$kg.m^{-3}$]	1700

2.3.5 Partition coefficients

In this section, the following processes are described:
- fraction of substance in air associated with aerosol
- partitioning between air and water
- partitioning between solids and water in soil, sediment, and suspended matter

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

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

Adsorption to aerosol particles

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

$$Fass_{aer} = \frac{CONjunge \bullet SURF_{aer}}{VP + CONjunge \bullet SURF_{aer}} \quad (5)$$

Explanation of symbols:

CONjunge	constant of Junge equation	[Pa.m]	*
$SURF_{aer}$	surface area of aerosol particles	[$m^2.m^{-3}$]	*
VP	vapour pressure	[Pa]	data set
$Fass_{aer}$	fraction of the chemical 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 & Hof, 1993).

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

$$VPL = \frac{VP}{e^{6.79 \bullet (1-\frac{TEMP_{melt}}{TEMP})}} \quad (6)$$

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

Volatilisation

The transfer of substances 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 $K_{air\text{-}water}$ (also known as the "dimensionless" Henry's Law constant) can be estimated from the ratio of the vapour pressure and the water solubility.

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

$$HENRY = \frac{VP \bullet MOLW}{SOL} \quad (7)$$

$$K_{air\text{-}water} = \frac{HENRY}{R \bullet TEMP} \quad (8)$$

Explanation of symbols:

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

Adsorption/desorption

Besides 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 and suspended matter can be obtained or estimated from:

- Direct measurement;
- Simulation testing;
- Koc measured by adsorption studies (OECD test guideline 106);
- Koc measured by HPLC-method (under development);
- Adsorption control of inherent biodegradability tests;
- If no Koc is available, it may be estimated from Kow (QSARs are given in Chapter 4).

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

If no measured data are available for a specific adsorbing material, it is assumed that all adsorption can be related to the organic matter of the medium, viz. standardisation to Koc (this is only valid for non-ionic substances) based on the organic carbon content of different media (e.g. soil, sediment, suspended matter, sewage sludge). For organic, non-ionic substances, Koc can be estimated from Kow as outlined in Chapter 4. The equation given for the class "predominantly hydrophobics" is preferred as default. For specific groups of substances, other QSARs are given.

The solid-water partition coefficient (Kp) in each compartment (soil, sediment, suspended matter) can be calculated from the Koc value, and the fraction organic carbon in the compartment. Initially, the fraction organic carbon from the standard environment should be used, as given in Table 3.

$$Kp_{comp} = Foc_{comp} \bullet Koc \qquad with\ comp \in \{soil, sed, susp\} \tag{9}$$

Explanation of symbols:

Koc	partition coefficient organic carbon-water	[l.kg^{-1}]	data set/Ch. 4
Foc_{comp}	weight fraction of organic carbon in compartment *comp*	[kg.kg^{-1}]	Table 3
Kp_{susp}	partition coefficient solid-water in suspended matter	[l.kg^{-1}]	
Kp_{sed}	partition coefficient solid-water in sediment	[l.kg^{-1}]	
Kp_{soil}	partition coefficient solid-water in soil	[l.kg^{-1}]	

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

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

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

$$with\ comp \in \{soil, susp, sed\} \tag{10}$$

Explanation of symbols:

$Fwater_{comp}$	fraction water in compartment *comp*	[$m^3.m^{-3}$]	Table 3
$Fsolid_{comp}$	fraction solids in compartment *comp*	[$m^3.m^{-3}$]	Table 3
$Fair_{comp}$	fraction air in compartment comp (only relevant for soil)	[$m^3.m^{-3}$]	Table 3
RHOsolid	density of the solid phase	[$kg.m^{-3}$]	2500
Kp_{comp}	solids-water part. coeff. in compartment *comp*	[l.kg^{-1}]	eq. (8)
$K_{air\text{-}water}$	air-water partitioning coefficient	[-]	eq. (7)
$K_{soil\text{-}water}$	soil-water partitioning coefficient	[$m^3.m^{-3}$]	
$K_{susp\text{-}water}$	suspended matter-water partitioning coefficient	[$m^3.m^{-3}$]	
$K_{sed\text{-}water}$	sediment-water partitioning coefficient	[$m^3.m^{-3}$]	

2.3.6 Biotic and abiotic 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. Since measured data on degradation processes for different compartments are usually not available, they must be extrapolated from standardised laboratory tests. In this section, degradation rate constants are derived for abiotic degradation (hydrolysis and photolysis) and biotic degradation (in soil, sediment, water, and sewage treatment). For hydrolysis and photolysis, only primary degradation is measured. In general, risk assessment focuses on the parent compound. Nevertheless, if stable degradation products are formed, these should be assessed as well.

Hydrolysis

Values for the half-life (DT50) of a hydrolysable substance can be converted to degradation rate constants, which may be used in the models for calculating PEC_{local} and especially $PEC_{regional}$. The results of a ready biodegradability study will show whether or not the hydrolysis products are themselves biodegradable. Similarly, for substances where DT50 is less than 12 hours, environmental effects are likely to be attributed to the hydrolysis products rather than to the parent substance itself. These effects should also be assessed. Similar principles may be applied to substances for which rapid photolysis has been demonstrated. QSAR methods are available for certain groups of substances (Chapter 4).

For many substances, the rate of hydrolysis will be heavily dependent on the specific environmental pH and temperature. For risk assessment purposes a pH of 7 and temperature of 285 K will normally be established which conform to the standard environmental parameters of Table 3. 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 or a hydrolysis product.

Where the use of an alternative pH would 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:

$$khydr_{water} = \frac{\ln 2}{DT50\,hydr_{water}} \quad (11)$$

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}]	

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). As there are no valid methods for estimating the quantum yield (see Chapter 4) the experimental determination of the quantum yield (OECD, 1992c) and the UV-absorption spectrum of the substance is a prerequisite for estimating the photodegradation in surface water. Due to high seasonal variation in light flux, photochemical processes should only be used in an averaged manner. Methods to derive average degradation rates which can be used in the model calculation of $PEC_{regional}$ are described in Zepp & Cline (1977) and Frank & 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 cases natural water bodies, the rate of photoreaction is affected by dissolved and suspended matter. Since the concentration of the chemical under consideration is normally low compared to the concentration of e.g. dissolved humic acids, by far the larger portion of the sunlight penetrating the water bodies is absorbed by the natural constituents.

Using the standard parameters of the regional model (water depth, suspended solids concentration), the reduction may be as large as 98%.

Indirect (sensitised) photochemical reactions should only be included in the over-all 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 & Klöppfer, 1989; GC-SOLAR by Zepp & Cline).

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

$$kphoto_{water} = \frac{\ln 2}{DT50\ photo_{water}} \qquad (12)$$

Explanation of symbols:

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

Photochemical reactions in the atmosphere

Although for some chemicals 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 $cm^3.molecule^{-1}.s^{-1}$) can either be determined experimentally (OECD, 1992c) or estimated by (Q)SAR-methods (see Chapter 4). By relating k_{OH} to the OH-radical concentration in the atmosphere, the pseudo-first order rate constant in air is determined:

$$kgd_{air} = k_{OH} \bullet OHCONC_{air} \bullet 24 \bullet 3600 \qquad (13)$$

Explanation of symbols:

k_{OH}	specific degradation rate constant with OH-radicals	[$cm^3.molec^{-1}.s^{-1}$]	data set/Ch.4
$OHCONC_{air}$	concentration of OH-radicals in atmosphere	[$molec.cm^{-3}$]	5.10^5 *
$kdeg_{air}$	pseudo first order rate constant for degradation in air	[d^{-1}]	

* The average OH-radical concentration over 24 hours in Western Europe can be assumed to be 5.10^5 $molecules.cm^{-3}$ (BUA, 1992).

Biodegradation in the sewage treatment plant

Most of the ready biodegradation tests that are used at the moment are aimed at measuring the mineralisation of a chemical. Hence, they give valuable information on the mineralisation of a substance and the possible formation of transformation products.

However, they do not give information on the primary degradation rate of the parent compound nor do they give a quantitative estimate of the removal percentage in a waste water treatment plant. Therefore, in order to make use of the biodegradation test results that are available and that are requested in the present chemical legislation, it is necessary to assign rate constants to the results of the standard tests that can be used 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 to be found. For the purpose of modelling a sewage treatment plant (STP), the rate constants of Table 4 were derived from the biodegradation screening tests. All constants in Table 4 have the following prerequisites:

- They are only used for the water dissolved fraction of the substance. Calculation of partitioning between water and sludge phases has been calculated prior to the application of the rate constant;
- Sufficiently valid data from internationally standardised tests are preferred;
- For some substances (e.g. certain detergents), higher biodegradation rates may be justified if this can be confirmed by experimental data.

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

Table 4 *Elimination in sewage treatment plants: Extrapolation from test results to rate constants in STP model (SimpleTreat)*

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

NOTES to Table 4:

(a) Ready biodegradability testing (28d) (92/69/EEC C.4 A-F, respectively, OECD 301 A-F (1992) or equivalent according to expert judgement)

The conditions used in ready biodegradation tests do not favour biodegradation because the ratio of test substance to micro-organisms is high and the number and/or type of competent organisms may be insufficient for metabolism of the substance.

The degree of 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 OECD Test Guidelines or the Annex V methods) 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 within the time window: in this case the substance would not be regarded as being readily biodegradable. If the chemical 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 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 the 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 not to be readily bio degradable, it is necessary to check whether it was inhibitory to microbial activity at the concentration level of the ready biodegradability test. If the substance is inhibitory, the ready biodegradation test may be conducted again at a non-inhibitory concentration, if possible.

(b) Inherent biodegradability testing (28d) (87/302/EEC, respectively, OECD 302 B-C (1981-1992) or equivalent according to expert judgement)

In tests for inherent biodegradability, the test conditions are designed to be more favourable to the micro-organisms 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 micro-organisms 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 time 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 chemical 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 were transformed into the following more specific criteria that the different inherent biodegradation tests must fulfil:

Zahn-Wellens test:	Pass level must be reached within 7 days, log-phase should be no longer than 3 days, percentage removal in the test before biodegradation occurs should be below 15 %.
MITI-II test:	Pass level must be reached within 14 days, log-phase should be no longer than 3 days.

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

Biodegradation in surface water, sediment and soil

The rate of biodegradation in surface water, soil and sediment is related to the structure of chemicals, 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 chemical is available for biodegradation.

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

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

Table 5 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. Kinetic criteria for the interpretation and use of inherent test results to assign a rate constant for removal in a sewage treatment plant were introduced to overcome the problem of extrapolation of infinite sludge retention times in inherent tests to limited time for growth in a sewage treatment (5- 20 days SRT). There is however no need to introduce these very same criteria for inherently biodegradable substances if degradation rates are to be assigned for the soil, sediment or surface water. The assigned residence time in these compartments (40 days to infinite) are longer than the test duration of inherent tests and therefore, kinetic criteria for the interpretation of the inherent test results may not be relevant. The assigned degradation half-lives of an inherent biodegradable of 150 days in surface water (Table 5) and 300 - 30000 days in soil and sediment (Table 6) will only affect the predicted regional concentration provided that the residence time of the chemical is much larger than the assigned half-life (i.e. only for chemicals present in soil compartment and sediment).

Table 5 *First order rate constants and half-lives for biodegradation in surface water based on results of screening tests on biodegradability*

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

In distribution models, calculations are performed for homogeneous compartments, i.e. sediment containing porewater and a solid phase, and soil containing air, porewater and a solid phase. Since it is assumed that no degradation takes place in the bound phase, the rate constant for the bulk sediment or soil in principle depends on the sediment/water or soil/water partition coefficient of the chemical. With increasing hydrophobicity (sorption) of the chemical, the fraction present in the porewater available for degradation decreases, and therefore the overall rate constant should also decrease. However, it was recognised that for substances with low Kp values at present not enough empirical data are available to assume some sort of dependence of the soil biodegradation half-life on the solids/water partition coefficient. Nevertheless, for substances with high Kp values there is evidence that some sort of Kp-dependence exists. Therefore degradation half-life classes for (bulk) soil, partly based on Kp were defined. Table 6 gives the half-lives for soil based on Kp values.

Table 6 *Half-lives for (bulk) soil based on results from standardised biodegradation test results*

	Half-life Soil (d)*		
Kp_{soil} [$l.kg^{-1}$]	**Ready**	**Ready, failing 10-d window**	**Inherent**
≤ 100	30	90	300
>100, ≤ 1000	300	900	3000
>1000, ≤ 10000	3000	9000	30000
etc.	etc.	etc.	etc.

* in case of non-biodegradable substances an infinite half-life is assumed.

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

$$kbio_{soil} = \frac{\ln 2}{DT50\,bio_{soil}} \qquad (14)$$

Explanation of symbols:

$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	Table 6
$kbio_{soil}$	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 chemical 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:

$$kbio_{sed} = \frac{\ln 2}{DT50\,bio_{soil}} \cdot Faer_{sed} \qquad (15)$$

Explanation of symbols:

$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	Table 6
$Faer_{sed}$	fraction of the sediment compartment that is aerobic	$[m^3.m^{-3}]$	0.10
$kbio_{sed}$	first order rate constant for degr. in bulk sediment	$[d^{-1}]$	

Simulation tests are available which, initially were developed for pesticides as guidelines of BBA (BBA, 1986; BBA, 1990a) and US EPA. When available, these test results should be evaluated on a case-by-case basis.

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 $PEC_{regional}$, the rate constants for these processes can be summed into one, overall degradation rate constant. It should be note that different types of degradation (primary and ultimate) are added. This is done for modelling purposes only. 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.

$$kdeg_{water} = khydr_{water} + kphoto_{water} + kbio_{water} \qquad (16)$$

Explanation of symbols:

$khydr_{water}$	first order rate constant for hydrolysis in surface water	$[d^{-1}]$	eq. (10)
$kphoto_{water}$	first order rate constant for photolysis in surface water	$[d^{-1}]$	eq. (11)
$kbio_{water}$	first order rate constant for biodegradation in surface water	$[d^{-1}]$	Table 5
$kdeg_{water}$	total first order rate constant for degradation in surface water	$[d^{-1}]$	

2.3.7 Elimination processes prior to the release to the environment

In this section, the following parameters are derived:
- emission from sewage treatment plant to air
- concentration in sewage sludge
- concentration in effluent of sewage treatment plant
- PEC for micro-organisms in 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. 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.

Waste water 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 waste water treatment plant and if yes, through which kind of treatment plant before being discharged into the environment. At the time of the writing of the TGD, the situation in the Member States concerning percentage connection to sewage works is quite diverse (see Appendix XII). Across the Community, taken as a whole, approximately 70% of the municipal waste water volume (domestic and industrial loads) is treated in a biological waste water treatment plant. In particular Article 4 of Council Directive 91/1271/EEC concerning urban waste water treatment requires Member States, before 31 December 2000, to ensure that municipal waste water discharged from agglomerations of more than 15,000 population equivalent is subject to biological (secondary) treatment before being discharged to the environment. In contrary, Article 6 allows Member States to declare non sensitive areas for which discharged waste water 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 (primarily). For a long time, the part of non-treated waste water in the EU will amount to 15 - 30 %.

The situation with respect to waste water treatment at industrial installations is less clear. It may be assumed that many of the larger industrial installations are either connected to a municipal waste water 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 waste water will pass through a STP before being discharged into the environment. Nevertheless, for the largest PEC_{local} 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 which 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 means of possible local risk reductions. The PEC without considering a STP-treatment will not be used in the exposure assessment, unless the substance considered has a specific use category where direct discharge to water is widely practised;
- For a standard regional scale environment (definition see section 2.3.8.1) it is assumed that 70% of the waste water is treated in a biological STP and the remaining 30% 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 waste water treatment plant is determined by the physico-chemical and biological properties of the substance (biodegradation, adsorption onto sludge, sedimentation of insoluble material, volatility) 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:

1. Measured data in full scale STP

The percentage removal should preferably be based upon measured influent and effluent concentrations. As with measured data in 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, rain retention capacity, etc. The data may be used provided that certain minimum criteria have been met, e.g. the measurements have been carried out over a longer period of time. Furthermore, consideration should be given to the fact that removal may be due to stripping or adsorption (not degradation). In case no mass balance study has been performed, the percentage of transport to air or sludge should be estimated, e.g. by scaling the fractions to air and sludge from the tables in Appendix II to the measured removal.

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

2. 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 waste water treatment plant or other environmental situations, for example a river. So far only the waste water treatment process can be studied in the laboratory by agreed methods, e.g. the Coupled Units Test (OECD, 1981). Removability is determined by monitoring the changes in DOC (Dissolved Organic Carbon) and/or COD (Chemical Oxygen Demand).

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

There is insufficient information available on the applicability of elimination data from the laboratory test to the processes of a real sewage plant. The results can be extrapolated to degradation in the real environment only if the concentrations that were used in the test are in the same order of magnitude than the concentrations that are to be expected in the real environment. If this is not the case, extrapolation can seriously overestimate the degradation rates especially when the extrapolation goes from high to low concentrations. If concentrations are in the same order of magnitude then the results of these tests can be used quantitatively to estimate the degree of removal of substances in a mechanical-biological STP.

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

3. Modelling STP

If there are no measured data available, the degree of removal can be estimated by means of a waste water treatment model using log Kow (Koc or more specific partition coefficients can also be used; see section 2.3.5), Henry's Law constant and the results of biodegradation tests as input parameters. However, it should be remembered that the distribution behaviour of transformation products are 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). With SimpleTreat, the sewage treatment plant is modelled as an average size treatment plant based on aerobic degradation by active sludge, and consisting of 9 compartments (see Figure 4). 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. 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.

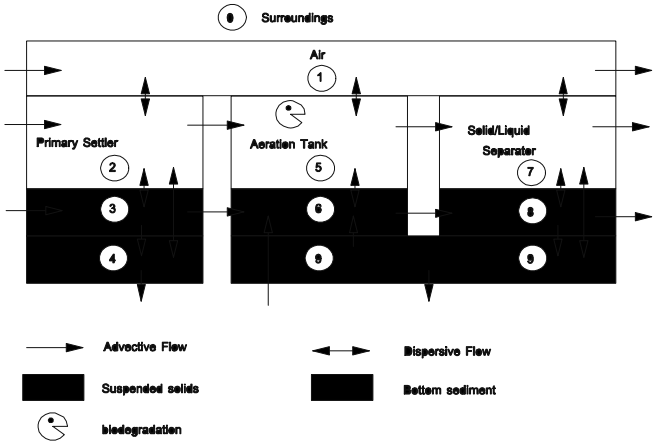

Figure 4 *Schematic design of the sewage treatment plant model SimpleTreat*

For the purpose of modelling a STP, the rate constants presented in Table 4 have been derived from the biodegradation screening tests. The modelling results from SimpleTreat using these first-order rate constants of 0, 0.1, 0.3 and 1 h^{-1} are tabulated in Appendix II. It contains relative emission data pertaining to air, water, and sludge as a function of Henry's Law constant and log Kow for the different biodegradation categories, according to Table 4. If no specific measured biodegradation rate data are available for the particular substance, the tabulated values from Appendix II should be used.

Typical characteristics of the standard sewage treatment plant are given in Table 7. The amount of surplus sludge per inhabitant equivalent and the concentration of suspended matter in influent are taken from SimpleTreat (run at low loading rate).

These values are the same as applied to derive the tables in Appendix II. At a higher tier in the risk assessment process more specific information on the biodegradation behaviour of a chemical 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 scenario's are optional:

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

Table 7 *Standard characteristics of a municipal sewage treatment plant*

Parameter	**Symbol**	**Unit**	**Value**
Capacity of the local STP	$CAPACITY_{stp}$	[eq]	10000
Capacity of the regional STP	$CAPACITYreg_{stp}$	[eq]	$2.0.10^{7}$
Capacity of the continental STP	$CAPACITYcon_{stp}$	[eq]	$3.7.10^{8}$
Amount of wastewater per inhabitant	WASTEWinhab	$[l.d^{-1}.eq^{-1}]$	200
Surplus sludge per inhabitant	SURPLUSsludge	$[kg.d^{-1}.eq^{-1}]$	0.011
Concentration susp. matter in influent	$SUSPCONC_{inf}$	$[kg.m^{-3}]$	0.45

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

Input

HENRY	Henry's law constant	$[Pa.m^3.mol^{-1}]$	eq. (6)
Kow	octanol-water partitioning coefficient	[-]	data set
$kbio_{stp}$	first-order rate constant for biodegradation in STP	$[d^{-1}]$	Table 4

Output

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

Calculation of the STP-influent concentration

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

$$Clocal_{inf} = \frac{Elocal_{water} \cdot 10^6}{EFFLUENT_{stp}} \quad (17)$$

Explanation of symbols:

$Elocal_{water}$	local emission rate to (waste) water during episode	[kg.d^{-1}]	eq. (2)
$EFFLUENT_{stp}$	effluent discharge rate of STP	[l.d^{-1}]	eq. (18)
$Clocal_{inf}$	concentration in untreated waste water	[mg.l^{-1}]	

Calculation of the STP-effluent concentration

The fraction of the chemical reaching the effluent of the STP is tabulated in Appendix II. The concentration of the effluent of the STP is given by the fraction to effluent and the concentration in untreated waste water as follows:

$$Clocal_{eff} = Clocal_{inf} \cdot Fstp_{water} \quad (18)$$

Explanation of symbols:

$Clocal_{inf}$	concentration in untreated waste water	[mg.l^{-1}]	eq. (16)
$Fstp_{water}$	fraction of emission directed to water by STP	[-]	App. II
$Clocal_{eff}$	concentration chemical in the STP-effluent	[mg.l^{-1}]	

if no specific data are known, $EFFLUENT_{stp}$ should be based on an averaged waste water flow of 200 l per capita per day for a population of 10,000 inhabitants (see Table 7):

$$EFFLUENT_{stp} = CAPACITY_{stp} \cdot WASTEWinhab \quad (19)$$

Explanation of symbols:

$CAPACITY_{stp}$	capacity of the STP	[eq]	Table 7
WASTEWinhab	sewage flow per inhabitant	[l.d^{-1}.eq^{-1}]	Table 7
$EFFLUENT_{stp}$	effluent discharge rate of STP	[l.d^{-1}]	

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

Calculation of the emission to air from the STP

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

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water} \quad (20)$$

Explanation of symbols:

$Fstp_{air}$	fraction of the emission to air from STP	[-]	App. II
$Elocal_{water}$	local emission rate to water during emission episode	[kg.d^{-1}]	eq. (2)
$Estp_{air}$	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:

$$C_{sludge} = \frac{Fstp_{sludge} \cdot Elocal_{water} \cdot 10^6}{SLUDGERATE} \quad (21)$$

Explanation of symbols:

$Elocal_{water}$	local emission rate to water during episode	[kg.d^{-1}]	eq. (2)
$Fstp_{sludge}$	fraction of emission directed to sludge by STP	[-]	App. II
SLUDGERATE	rate of sewage sludge production	[kg.d^{-1}]	eq. (21)
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:

$$SLUDGERATE = \frac{2}{3} \cdot SUSPCONC_{inf} \cdot EFFLUENT_{stp} + SURPLUSsludge \cdot CAPACITY_{stp} \quad (22)$$

Explanation of symbols:

$SUSPCONC_{inf}$	concentration of susp. matter in STP influent	[kg.m^{-3}]	Table 7
$EFFLUENT_{stp}$	effluent discharge rate of STP	[m^3.d^{-1}]	eq. (18)
SURPLUSsludge	surplus sludge per inhabitant equivalent	[kg.d^{-1}.eq^{-1}]	Table 7
$CAPACITY_{stp}$	capacity of the STP	[eq]	Table 7
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 micro-organisms

Some substances have an adverse impact on microbial activity. For the risk characterisation of a chemical upon micro-organisms in the STP, ideally the concentration in the aeration tank should be used. Assuming homogeneous mixing in the aeration tank, the dissolved concentration of a substance there is equal to the effluent concentration:

$$PEC_{stp} = Clocal_{eff} \quad (23)$$

Explanation of symbols:

$Clocal_{eff}$	total concentration of chemical in STP effluent	$[mg.l^{-1}]$	eq. (17)
PEC_{stp}	PEC for micro-organisms in the STP	$[mg.l^{-1}]$	

However, in the case of intermittent release, the concentration in influent of the STP is more representative:

$$PEC_{stp} = Clocal_{inf} \quad (24)$$

Explanation of symbols:

$Clocal_{inf}$	total concentration of chemical in STP influent	$[mg.l^{-1}]$	eq. (16)
PEC_{stp}	PEC for micro-organisms in the STP	$[mg.l^{-1}]$	

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 micro-organisms. In modern waste water 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 following parameters are derived:
- local PECs for all environmental compartments
- regional PECs for all environmental compartment

2.3.8.1 Introduction

In the following sections guidance is given for the calculation of the PEC_{local} for each compartment. In section 2.3.8.7, the calculation of regional steady-state concentrations ($PEC_{regional}$) in each compartment is presented. Table 8 presents an overview of the PECs that need to be estimated.

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

- The concentration in surface water ($PEClocal_{water}$) is in principle calculated after complete mixing of the effluent outfall. Because of the short time between effluent discharge and exposure location, dilution will usually be the dominant "removal" process. Therefore, degradation in surface water, 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 chemical that is adsorbed to suspended matter. The resulting dissolved concentration is used for comparison with $PNEC_{water}$ (section 2.3.8.3). The concentration in sediment is calculated at the same location. For exposure of aquatic organisms, having a relatively short lifespan, the concentration during an emission episode is calculated. For indirect exposure of humans and predating birds and mammals, annual averages are used, being more appropriate with respect to chronic exposure;
- The concentration in soil ($PEClocal_{soil}$) is calculated as an average concentration over a certain time-period in agricultural soil, fertilised with sludge from a STP and receiving continuous aerial deposition from a nearby point source (section 2.3.8.5) (production/processing site and STP aeration tank). Two different soil types are distinguished: arable land and grassland, which differ in the amount of sludge applied, and the mixing depth. For the terrestrial ecosystem, the concentration is averaged over 30 days, for human indirect exposure a period of 180 days is used. The concentration in groundwater is calculated below this agricultural area;
- The concentration in air ($PEClocal_{air}$) is calculated as an average concentration at 100 meters from the source. This distance is assumed to be representative for the average size of an industrial site. Deposition is calculated as an average for a circle around the source with a radius of 1000 m which is supposed to represent the local agricultural area (section 2.3.8.2). Deposition is used as input for the soil module, annual average deposition fluxes are used. The concentration in air is used for exposure of humans, therefore, an annual average concentration is calculated;
- The regional standard environment is assumed to be highly industrialised, relatively small but densely populated; the size is 200x200 km with 20 million inhabitants. It is assumed that 10% of the European production takes place within this area (section 2.3.8.7). Emissions are assumed to be a continuous and diffuse flux into the environment.

Other pathways than those described, like the release to air, to surface water and to soil from waste disposal sites or deposition from air to surface waters, could be of relevance. No guidance for those pathways is currently available. In addition, releases into sea or estuarine waters are not considered specifically.

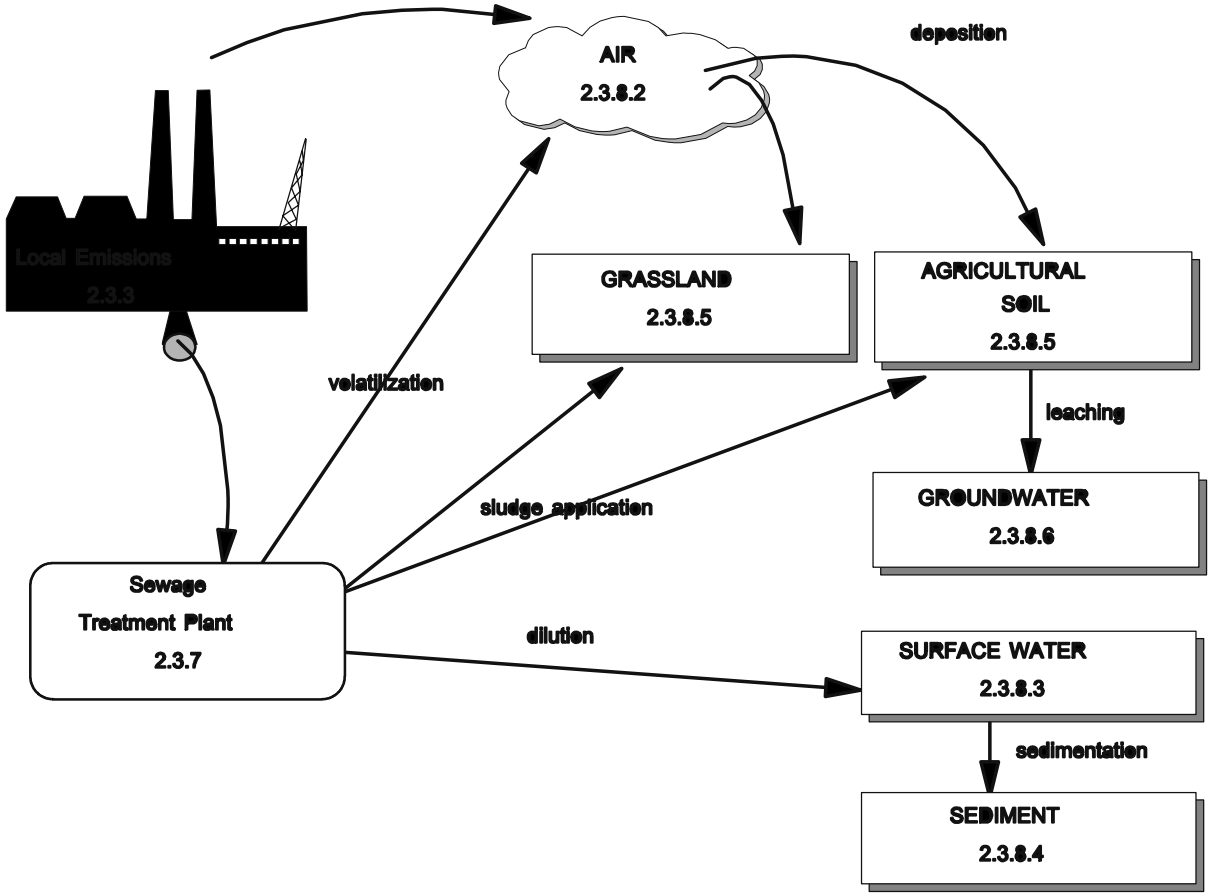

Figure 5 *Local relevant emission and distribution routes*

Figure 5 shows the relationship between the local emission routes and the subsequent distribution processes which may be relevant for the different environmental compartments. For each compartment, specific fate and distribution models are applied.

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

Table 8 *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 a 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 agricultural 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
Micro-organisms	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 fate processes that are possible in air, are schematically drawn in Figure 6.

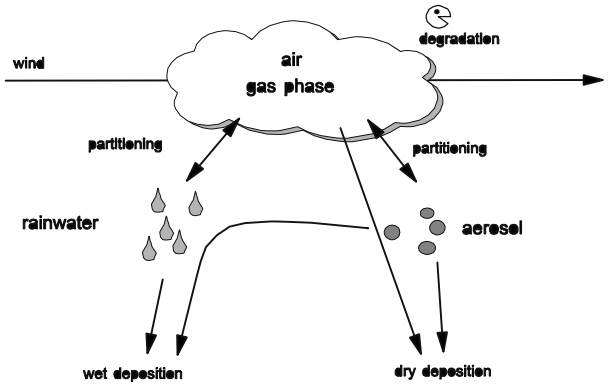

Figure 6 *Possible fate processes in the air compartment*

PEC_{local} for air cannot be compared with the PNEC for air because the latter is not available. The PEC_{local} for air is used as input for the calculation 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.

Many air models are available that are highly flexible and can be adjusted to take specific information on scale, emission sources, weather conditions etc. into account. For new chemicals, as well as very often for existing chemicals, 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 chemicals is calculated separately. The partitioning between gas and aerosol is determined by means of the equation of Junge (see equation (5));

- The atmospheric reaction rate is set at a fixed value of 5% per hour. However, on the spatial scale that is regarded, atmospheric reactions do not play any role in the removal of the substance (even at very high reaction rates) (Toet and De Leeuw, 1992);
- Losses due to deposition are neglected for estimation of the concentration and deposition fluxes at this short distance from the source;
- Assumed source characteristics are:
  - source height: 10 meters, representing the height of buildings in which production, processing or use take place;
  - heat content of emitted gases: 0; this assumes there is no extra plume rise caused by excess heat of vapours compared to the outdoor temperature;
  - source area: 0 meter; representing an ideal point source which is obviously not always correct but which is an acceptable choice;
- Calculated concentrations are long-term averages.

The concentration in air at a distance of 100 meters from the point source is estimated. This distance is chosen to represent the average distance between the emission source and the border of the industrial site. The deposition flux of gaseous and aerosol-bound chemicals 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 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}:

$$Clocal_{air} = \max\left(Elocal_{air} , Estp_{air} \right) \cdot Cstd_{air} \quad (25)$$

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365} \quad (26)$$

Explanation of symbols:

$Elocal_{air}$	local direct emission rate to air during episode	[kg.d^{-1}]	eq. (2)
$Estp_{air}$	local indirect emission to air from STP during episode	[kg.d^{-1}]	eq. (19)
$Cstd_{air}$	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}]	

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air} \quad (27)$$

Explanation of symbols:

$Clocal_{air,ann}$	annual average local concentration in air	[mg.m^{-3}]	eq. (25)
$PECregional_{air}$	regional concentration in air	[mg.m^{-3}]	2.3.8.7
$PEClocal_{air,ann}$	annual average predicted environmental conc. in air	[mg.m^{-3}]	

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

$$DEPtotal = \left(Elocal_{air} + Estp_{air} \right) \cdot \left(Fass_{aer} \cdot DEPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right) \quad (28)$$

$$DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365} \quad (29)$$

Explanation of symbols:

$Elocal_{air}$	local direct emission rate to air during emission episode	[kg.d^{-1}]	eq. (2)
$Estp_{air}$	local indirect emission to air from STP during episode	[kg.d^{-1}]	eq. (19)
$Fass_{aer}$	fraction of the chemical bound to aerosol	[-]	eq. (5)
$DEPstd_{aer}$	standard deposition flux of aerosol-bound compounds at a source strength of 1 kg.d^{-1}	[mg.m^{-2}.d^{-1}]	1.10^{-2}
$DEPstd_{gas}$	deposition flux of gaseous compounds as a function of Henry's Law coefficient, at a source strength of 1 kg.d^{-1}	[mg.m^{-2}.d^{-1}]	
	^{10}logHENRY ≤ -2:		5.10^{-4}
	-2 < ^{10}logHENRY ≤ 2:		4.10^{-4}
	^{10}logHENRY > 2:		3.10^{-4}
Temission	number of days per year that the emission takes place	[d.yr^{-1}]	App. IB
DEPtotal	total deposition flux during emission episode	[mg.m^{-2}.d^{-1}]	
$DEPtotal_{ann}$	annual average total deposition flux	[mg.m^{-2}.d^{-1}]	

2.3.8.3 Calculation of PEC_{local} for the aquatic compartment

In this section, the following parameters are derived:
- local concentration in surface water during emission episode
- annual average local concentration in surface water

The effluent of the sewage treatment plant is diluted into the surface water. Figure 7 shows the possible fate processes of the aquatic compartment. For the calculations, the following assumptions are made:

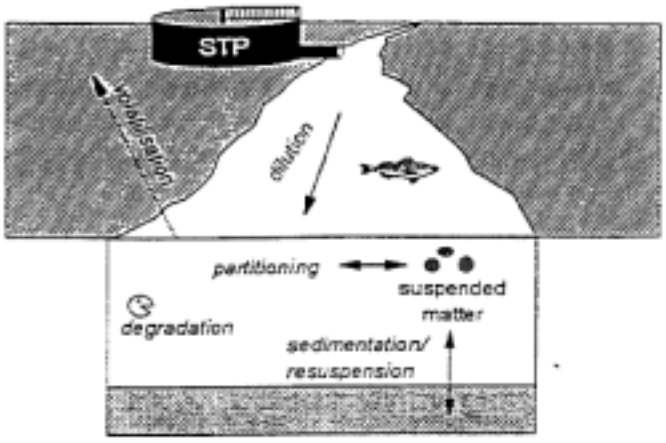

Figure 7 *Possible fate processes in surface water*

- Complete mixing of the effluent in the surface water is assumed as a representative exposure situation for the aquatic ecosystem;
- 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.

The calculation of the PEC_{local} for the aquatic compartment involves several sequential steps (see also Figure 5). 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 & de Nijs, 1990). The dilution factor is generally linked to the release scenario of the use category. For example, for consumer products an average dilution factor for sewage from municipal treatment plants of 10 is recommended. This is also regarded as a default dilution value for other types of substance if no specific data are available.

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 local distribution models can be used.

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

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

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

The local concentration in surface water is calculated as follows.

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION} \qquad (30)$$

Explanation of symbols:

$Clocal_{eff}$	concentration of the chemical in the STP-effluent	$[mg.l^{-1}]$	eq. (17)
Kp_{susp}	solids-water partitioning coefficient of suspended matter	$[l.kg^{-1}]$	eq. (8)
$SUSP_{water}$	concentration of suspended matter in the river	$[mg.l^{-1}]$	15
DILUTION	dilution factor	[-]	10
$Clocal_{water}$	local concentration in surface water during emission episode	$[mg.l^{-1}]$	

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

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}} \quad (31)$$

Explanation of symbols:

$EFFLUENT_{stp}$	effluent discharge rate of stp	[$l.d^{-1}$]	eq. (18)
FLOW	flow rate of the river	[$l.d^{-1}$]	data set
DILUTION	dilution factor at the point of complete mixing	[-]	

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

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365} \quad (32)$$

Explanation of symbols:

$Clocal_{water}$	local concentration in surface water during emission episode	[$mg.l^{-1}$]	eq. (29)
Temission	number of days per year that the emission takes place	[$d.yr^{-1}$]	App. IB
$Clocal_{water,ann}$	annual average local concentration in surface water	[$mg.l^{-1}$]	

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

$$PEClocal_{water} = Clocal_{water} + PECregional_{water} \quad (33)$$

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECregional_{water} \quad (34)$$

Explanation of symbols:

$Clocal_{water}$	local concentration in surface water during episode	[$mg.l^{-1}$]	eq. (29)
$Clocal_{water,ann}$	annual average concentration in surface water	[$mg.l^{-1}$]	eq. (31)
$PECregional_{water}$	regional concentration in surface water	[$mg.l^{-1}$]	2.3.8.7
$PEClocal_{water}$	predicted environmental concentration during episode	[$mg.l^{-1}$]	
$PEClocal_{water,ann}$	annual average predicted environmental concentration	[$mg.l^{-1}$]	

2.3.8.4 Calculation of PEC_{local} for sediment

In this section, the following parameters are derived:
- local concentration in sediment during 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 thermodynamical partition equilibrium (see also Di Toro et al., 1991):

$$PEClocal_{sed} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water} \cdot 1000 \qquad (35)$$

Explanation of symbols:

$PEClocal_{water}$	concentration in surface water during emission episode	[$mg.l^{-1}$]	eq. (32)
$K_{susp\text{-}water}$	suspended matter-water partitioning coefficient	[$m^3.m^{-3}$]	eq. (9)
RHO_{susp}	bulk density of suspended matter	[$kg.m^{-3}$]	eq. (4)
$PEClocal_{sed}$	predicted environmental concentration in sediment	[$mg.kg^{-1}$]	

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

2.3.8.5 Calculation of PEC_{local} for the soil compartment

In this section, the following parameters are derived:
- local concentration in agricultural soil (averaged over a certain time period)
- local concentration in grassland (averaged over a certain time period)
- percentage of steady-state situation (to indicate persistency)

Exposure assessment for the soil compartment is important with respect to exposure of terrestrial organisms. Furthermore, crops are grown on agricultural soils for human consumption, and cattle, producing meat and milk, is grazing on grasslands. Figure 8 shows the possible fate processes in the soil compartment.

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.

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

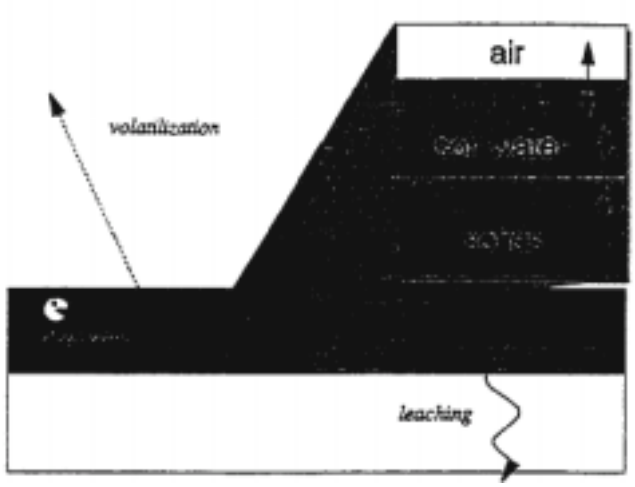

Figure 8 *Possible fate processes in the soil compartment.*

For sludge application to agricultural soil an application rate of 5000 kg/ha dry weight per year is assumed while for grassland a rate of 1000 kg/ha/yr should be used. Sludge application is treated as a single event once a year. The contribution to the overall impact from wet and dry deposition is based on the emission calculation of a point source (section 2.3.8.2) and is related to a surrounding area within 1000 m from that source.

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 correct since the deposition flux is linked to the emission episode. Averaging is done to facilitate calculation of a steady-state level. Furthermore, it is impossible to indicate when the emission episode takes place in a year: in the beginning of the growing season, the impact on exposure levels will be large, after the growing season, the impact will be insignificant. Therefore, averaging represents an appropriate scenario choice.

The PEC in agricultural soil is used for two purposes:

- Characterisation of risk to terrestrial ecosystems (section 4);
- Starting point for calculation of indirect exposure to humans via crops and cattle products (see Chapter 2: Risk Assessment for Human Health).

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

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

$$\frac{dC_{soil}}{dt} = - k \cdot C_{soil} + D_{air} \qquad (36)$$

Explanation of symbols:

D_{air}	aerial deposition flux per kg of soil	[mg.kg^{-1}.d^{-1}]	eq. (36)
t	time	[d]	
k	first order rate constant for removal from top soil	[d^{-1}]	eq. (40)
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:

$$D_{air} = \frac{DEPtotal_{ann}}{DEPTH_{soil} \cdot RHO_{soil}} \qquad (37)$$

Explanation of symbols:

$DEPtotal_{ann}$	annual average total deposition flux	[mg.m^{-2}.d^{-1}]	eq. (28)
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 9
RHO_{soil}	bulk density of soil	[kg.m^{-3}]	eq. (4)
D_{air}	aerial deposition flux per kg of soil	[mg.kg^{-1}.d^{-1}]	

The differential equation (35) has an analytical solution, given by:

$$C_{soil}(t) = \frac{D_{air}}{k} - \left[\frac{D_{air}}{k} - C_{soil}(0) \right] \cdot e^{-k\,t} \qquad (38)$$

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

Accumulation of the substance may occur when sludge is applied over consecutive years. This is illustrated in Figure 9. As a realistic worst-case exposure scenario, sludge is assumed to be 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 9, the concentration in soil is not constant in time.

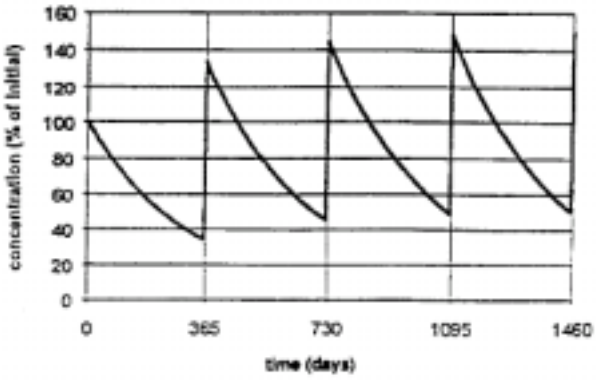

Figure 9 *Accumulation in soil due to several years of sludge application*

The concentration will be high just after sludge application (in the beginning of the growing 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 exposure to man, it is more appropriate to use an extended period of 180 days.

This averaging procedure is illustrated in Figure 10 (the average concentration is given by the area of the shaded surface, divided by the number of days).

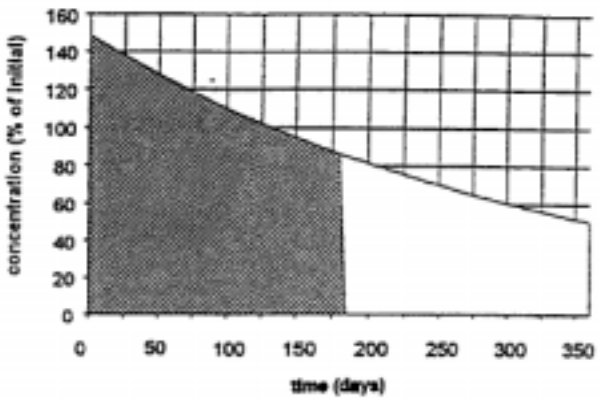

Figure 10 *The concentration in soil after 10 years. The shaded area is the integrated concentration over a period of 180 days*

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:

$$Clocal_{soil} = \frac{1}{T} \cdot \int_0^T C_{soil}\,(t)\,dt \qquad (39)$$

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

$$Clocal_{soil} = \frac{D_{air}}{k} + \frac{1}{k\,T}\left[\, C_{soil}\,(0) - \frac{D_{air}}{k} \,\right] \cdot \left[1 - e^{-k\,T}\right] \qquad (40)$$

Explanation of symbols:

D_{air}	aerial deposition flux per kg of soil	[mg.kg^{-1}.d^{-1}]	eq. (36)
T	averaging time	[d]	Table 9
k	first order rate constant for removal from top soil	[d^{-1}]	eq. (40)
C_{soil} (0)	initial concentration (after sludge application)	[mg.kg^{-1}]	eq. (47)
$Clocal_{soil}$	average concentration in soil over T days	[mg.kg^{-1}]	

Derivation of the removal rate constants

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

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

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

$$k = k_{volat} + k_{leach} + kbio_{soil} \qquad (41)$$

Explanation of symbols:

k_{volat}	pseudo-first order rate constant for volatilisation from soil	[d^{-1}]	eq. (41)
k_{leach}	pseudo-first order rate constant for leaching from top soil	[d^{-1}]	eq. (42)
$kbio_{soil}$	pseudo-first order rate constant for biodegradation in soil	[d^{-1}]	Table 6
k	first order rate constant for removal from top soil	[d^{-1}]	

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

$$\frac{1}{k_{volat}} = \left(\frac{1}{kasl_{air} \cdot K_{air\text{-}water}} + \frac{1}{kasl_{soilair} \cdot K_{air\text{-}water} + kasl_{soilwater}} \right) \cdot K_{soil\text{-}water} \cdot DEPTH_{soil} \qquad (42)$$

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
$kasl_{soilwater}$	partial mass transfer coeff. at soilwater-side of the air-soil int.	[$m.d^{-1}$]	$4.8 \cdot 10^{-5}$
$K_{air\text{-}water}$	air-water equilibrium distribution constant	[$m^3.m^{-3}$]	eq. (7)
$K_{soil\text{-}water}$	soil-water partitioning coefficient	[$m^3.m^{-3}$]	eq. (9)
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 9
k_{volat}	pseudo first-order rate constant for volatilisation from soil	[d^{-1}]	

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

$$k_{leach} = \frac{Finf_{soil} \cdot RAINrate}{K_{soil\text{-}water} \cdot DEPTH_{soil}} \quad (43)$$

Explanation of symbols:

$Finf_{soil}$	fraction of rain water that infiltrates into soil	[-]	0.25
RAINrate	rate of wet precipitation (700 mm/year)	$[m.d^{-1}]$	$1.92 \cdot 10^{-3}$
$K_{soil\text{-}water}$	soil-water partitioning coefficient	$[m^3.m^{-3}]$	eq. (9)
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 9
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 was 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 (39)), 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 (37) with an initial concentration of zero and 10 years of input:

$$Cdep_{soil\,10}(0) = \frac{D_{air}}{k} - \frac{D_{air}}{k} \cdot e^{-365 \cdot 10 \cdot k} \quad (44)$$

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:

$$Csludge_{soil\,1}(0) = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO_{soil}} \quad (45)$$

Explanation of symbols:

C_{sludge}	concentration in dry sewage sludge	$[mg.kg^{-1}]$	eq. (20)
$APPL_{sludge}$	dry sludge application rate	$[kg.m^{-2}.yr^{-1}]$	Table 9
$DEPTH_{soil}$	mixing depth of soil	[m]	Table 9
RHO_{soil}	bulk density of soil	$[kg.m^{-3}]$	eq. (4)
$Csludge_{soil\,1}(0)$	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:

$$Facc = e^{-365\,k} \tag{46}$$

Explanation of symbols:

k	first order rate constant for removal from top soil	[d^{-1}]	eq. (40)
Facc	fraction accumulation in one year	[-]	

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

$$Csludge_{soil\,10}\,(0) = Csludge_{soil\,1}\,(0) \cdot \left[1 + \sum_{n=1}^{9} Facc^{n} \right] \tag{47}$$

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

$$C_{soil\,10}\,(0) = Cdep_{soil\,10}\,(0) + Csludge_{soil\,10}\,(0) \tag{48}$$

This initial concentration can be used in equation (39) 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 substance may accumulate for hundreds of years. To indicate potential problems of persistency in soil, the fraction of the steady-state concentration can be derived:

$$Fst\text{-}st = \frac{C_{soil\,10}\,(0)}{C_{soil\,\infty}\,(0)} \tag{49}$$

Explanation of symbols:

$C_{soil\,10}\,(0)$	initial concentration after 10 years	[$mg.kg^{-1}$]	eq. (47)
$C_{soil\,\infty}\,(0)$	initial concentration in steady-state situation	[$mg.kg^{-1}$]	eq. (49)
Fst-st	fraction of steady-state in soil achieved	[-]	

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

$$C_{soil\,\infty}\,(0) \;=\; \frac{D_{air}}{k} \;+\; Csludge_{soil\,1}\,(0) \;\cdot\; \frac{1}{1 \;-\; Facc} \qquad (50)$$

Explanation of symbols:

D_{air}	aerial deposition flux per kg of soil	[mg.kg^{-1}.d^{-1}]	eq. (36)
k	first order rate constant for removal from top soil	[d^{-1}]	eq. (40)
Facc	fraction accumulation in one year	[-]	eq. (45)
$Csludge_{soil\,1}$ (0)	concentration in soil due to sludge in first year at t=0	[mg.kg^{-1}]	eq. (44)
$C_{soil\infty}$(0)	initial concentration in steady-state situation	[mg.kg^{-1}]	

Calculation of $PEClocal_{soil}$

For soil, three different PECs are calculated, for different endpoints (Table 9).

Table 9 *Characteristics of soil and soil-use for the three different endpoints.*

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

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

The concentration at the regional scale is used as background concentration for the local scale. It should be noted that, 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.

$$PEClocal_{soil} = Clocal_{soil} + PECregional_{natural\ soil} \quad (51)$$

Explanation of symbols:

$Clocal_{soil}$	local concentration in soil	[mg.kg^{-1}]	eq. (39)
$PECregional_{natural\ soil}$	regional concentration in natural soil	[mg.kg^{-1}]	2.3.8.7
$PEClocal_{soil}$	predicted environmental conc. in soil	[mg.kg^{-1}]	

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

$$PEClocal_{soil,porew} = \frac{PEClocal_{soil} \cdot RHO_{soil}}{K_{soil\text{-}water} \cdot 1000} \quad (52)$$

Explanation of symbols:

$PEClocal_{soil}$	predicted environmental conc. in soil	[mg.kg^{-1}]	eq. (50)
$K_{soil\text{-}water}$	soil-water partitioning coefficient	[m^3.m^{-3}]	eq. (9)
RHO_{soil}	bulk density of wet soil	[kg.m^{-3}]	eq. (4)
$PEClocal_{soil,porew}$	predicted environmental conc. in porewater	[mg.l^{-1}]	

2.3.8.6 Calculation of concentration in groundwater

In this section, the following parameters are derived:
- local concentration in groundwater

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

$$PEClocal_{grw} = PEClocal_{agr.soil,porew} \quad (53)$$

Explanation of symbols:

$PEClocal_{agr.soil,porew}$	predicted environmental conc. in porewater	[mg.l^{-1}]	eq. (51)
$PEClocal_{grw}$	predicted environmental conc. in groundwater	[mg.l^{-1}]	

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) and by Van de Meent, (1993) (SimpleBox).

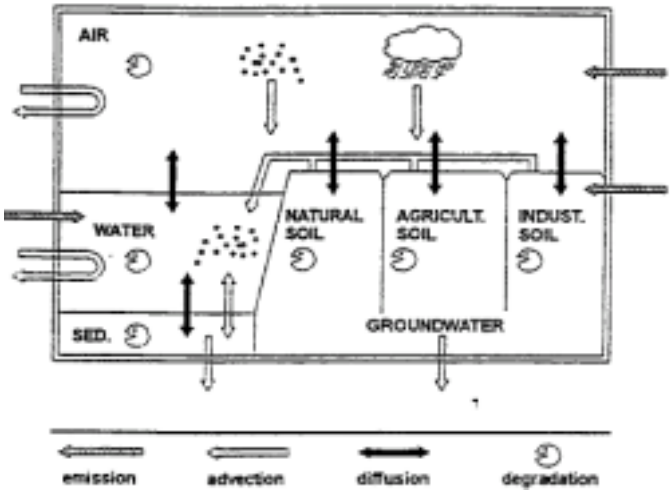

Figure 11 *The relevant emission and distribution routes*

These models are box models, consisting of a number of compartments (see Figure 11) which are considered homogeneous and well mixed. A chemical released into the model is distributed between the compartments according to the properties of both the chemical and the model environment. Several types of fate processes are distinguished in the regional assessment, as drawn in Figure 11:

- 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 chemical 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.

Chemical 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 chemical at the "border" of the region must be taken into account. This is defined as the background concentration of a chemical. The background concentration in a local model can be obtained from the outcome of the regional model. For chemicals 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 chemical 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 70% (the EU average according to Appendix XII) will be assumed.

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

Model parameters for $PEC_{regional}$

When calculating the $PEC_{regional}$ it is important which modelling parameters are chosen and what fraction of the total emission 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 x 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 10. 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 10 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 3.

Table 10 *Proposed model parameters for regional model*

Parameter	**Value in regional model**
area of the regional system	$4 \cdot 10^4$ 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	70%

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 (Agrostat data-base). 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 flow of water through the system is the sum of the amount of rain (run off and directly into surface water), effluent discharges, and inflow of rivers. Given the average annual rainfall of 700 mm and a runoff fraction of 0.25, the resulting flow of water through the model environment necessary to obtain this residence time is $6.9 \cdot 10^7$ m^3.d^{-1}.

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

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 11.

Table 11 *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 has the size of all EU countries together (Norway included) and similar percentages for water and natural, agricultural and industrial/urban soils as given in Table 10. These values are summarised in Table 12. 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 chemical. 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. It is assumed that no inflow of the substance into the continental system takes place.

Table 12 *Parameters for continental model*

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

2.4 Summary of PECs derived

Summarised, the local estimations yield the following input and output information:

Input

Physico-chemical properties	section 2.3.2
Characterisation of the environment	Table 3
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

$PEC_{micro\text{-}organisms}$	local PEC for micro-organisms in the STP	[mg.l^{-1}]	eq. (22), (23)
$PEClocal_{water}$	local PEC in surface water (dissolved) during episode	[mg.l^{-1}]	eq. (32)
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	[mg.l^{-1}]	eq. (33)
$PEClocal_{sed}$	local PEC in sediment (total)	[mg.kg^{-1}]	eq. (34)
$PEClocal_{air,ann}$	annual average local PEC in air (total)	[mg.m^{-3}]	eq. (26)
$PEClocal_{soil}$	local PEC in agricultural soil (total), averaged over 30 days	[mg.kg^{-1}]	eq. (50)
$PEClocal_{agr.soil}$	local PEC in agricultural soil (total), averaged over 180 days	[mg.kg^{-1}]	eq. (50)
$PEClocal_{grassland}$	local PEC in grassland (total), averaged over 180 days	[mg.kg^{-1}]	eq. (50)
$PEClocal_{agr.soil,porew}$	local PEC in porewater of agricultural soil	[mg.l^{-1}]	eq. (51)
$PEClocal_{grassland,porew}$	local PEC in porewater of grassland	[mg.l^{-1}]	eq. (51)
$PEClocal_{grw}$	local PEC in groundwater under agricultural soil	[mg.l^{-1}]	eq. (52)

Summarised, the regional estimations yield the following input and output information:

Input

Physico-chemical properties	section 2.3.2
Characterisation of the environment	Table 3
Parameters of the regional compartments	Table 10, Table 11, Table 12
Emission data	section 2.3.3.3
Partitioning coefficients	section 2.3.5
Degradation rates	section 2.3.6
Fate in sewage treatment plants	section 2.3.7

Output

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

2.5 Decision on the environmental concentration used for risk characterisation

When PECs have been derived from both measured data and calculation, they are compared. If they are not of the same order of magnitude (calculated PEC ≈ PEC based on measured concentrations), analysis and critical discussion of divergences are important steps for developing an environmental risk assessment of existing chemicals. 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 monitoring data might represent the background concentration or $PEC_{regional}$ in the regarded environmental compartment. If the calculated PEC is larger than the detection limit, but the measured data are below, then the detection limit should be used in the risk characterisation, taking the above mentioned arguments into account;

- 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 disregarded when calculating the PEC. An alternative cause could be a recent change in use pattern or emission reducing measures which are not yet reflected in the PEC based on measured concentrations.

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 stable metabolite of another substance;
- a retarded remobilization results from a pool present in other environmental compartments (e.g. from scrap or waste materials or former applications).

If the measured values have passed the procedure of critical statistical and geographical evaluation, a high degree of confidence can be attributed to those data and they shall overwrite the calculated PECs.

3. Effects assessment

3.1 Introduction

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

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

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

As stated in section 1.2, the protection goals for the environment are the aquatic and terrestrial ecosystem, top predators, microbial activity in a STP, and the atmosphere. This means that for each of these goals a PNEC has to be derived. A PNEC is regarded as a concentration below which an unacceptable effect will most likely not occur. In principle, the PNEC is calculated by dividing the lowest short term $L(E)C_{50}$ or long term NOEC value by an appropriate assessment factor. The assessment factors reflect the degree of uncertainty in extrapolation from laboratory toxicity test data for a limited number of species to the 'real' environment. Assessment factors applied for long-term tests are smaller as the uncertainty of the extrapolation from laboratory data to the natural environment is reduced. For this reason long-term data are preferred to short-term data.

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

The microbial activity in domestic STPs may be affected. Assessment factors to derive a $PNEC_{micro\text{-}organisms}$ are given in section 3.4.

Probably for most compounds no data will be present for sediment-dwelling organisms. Appropriate test systems are under development but standardised guidelines are not yet available. A method to compensate for this lack of toxicity data is used to derive a $PNEC_{sed}$; the equilibrium partitioning method (see section 3.5).

Also for the soil compartment few toxicity data are available. Where such data are present, they will normally include only short-term studies. If data are lacking, the equilibrium partitioning method can be used to derive a $PNEC_{soil}$. Otherwise, assessment factors are applied (see section 3.6).

For the atmosphere biotic and abiotic effects like acidification are addressed. Considering the lack of suitable data and as no adequate methods are available yet to assess both types of effects, a provisional strategy is described in section 3.7.

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

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

3.2 Evaluation of data

3.2.1 Ecotoxicity data

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

3.2.1.1 Completeness of data

New substances

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

Existing substances

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

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

3.2.1.2 Adequacy of data

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

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

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

The assessment of data adequacy involves therefore a review of individual data elements with respect to how the study is conducted and how the results are interpreted and a critical selection (and rejection) of data in its proper context and in accordance with the purpose of the assessment.

New substances

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

Existing substances

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

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

Whenever studies carried out according to current methods (e.g. EC, OECD, or EPA) are available, greater weight should normally be attached to them (Ahlers et al., 1992; Water Quality Institute, Denmark). On this background, the criteria for the reliability of a test are concentrated to the question whether sufficient information on the test is available and whether the investigations were carried out according to the generally accepted standards. The following possibilities exist:

- A complete test report is available or the test has been described in sufficient detail and the test procedure is in accordance with generally accepted scientific standards. These data are considered valid and can be used for risk assessment;
- The validity of the data cannot fully be established or the test differs in some respects from the test guidelines and the generally accepted scientific standards. Experts must decide in each case whether the test will be taken into consideration in the risk assessment or is regarded as not valid;
- It is obvious that the data are not valid because critical pieces of information are not available (e.g. it is not possible to establish the identity of the test substance).

These data are considered not valid and should not be used for the risk assessment. However, they may be used to design an appropriate test.

In principle, the same criteria apply for tests reported in published literature. The amount of information presented will provide the basis to decide on the quality of a report. In general, publications in peer reviewed journals are preferable. High quality reviews may be used as supporting information. Summaries or abstract publications may also supply supporting material.

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

Results from field studies may also be available. These studies can vary in experimental design: from indoor microcosms to outdoor macrocosms like experimental streams (Hill et al., 1994). Field studies may provide a better insight into the effects (including indirect effects), as well as routes of exposure (e.g. bioavailability, biodegradation) of the chemical considered. At present, there are no internationally accepted guidelines for field tests. However, some general guidance has been given for field studies with aquatic ecosystems (SETAC, 1991; SETAC, 1992).

Relevance of data

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

Interpretation of data

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

Short-term $L(E)C_{50}$ and long-term NOEC values are used in the effects assessment. However, results from ecotoxicological studies may be reported in a different way. In Table 13 guidance is given with respect to the derivation of $L(E)C_{50}$ and NOEC values.

In assessing long term aquatic toxicity tests with very hydrophobic organic chemicals such as PCBs, QSARs may be helpful. Due to their low water solubility, long term tests with such chemicals are difficult to perform as stable test concentrations are difficult to maintain. Also, it may take very long to reach steady state in the test organisms due to their low elimination rate. By comparing the test result with the "minimum toxicity" using the log Kow of the compound, insight can be gained into the validity of the test (see Chapter 4 on the "Use of QSARs").

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

3.2.2 Quantitative Structure-Activity Relationships

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

Table 13 *Different 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 less than three values between the $L(E)C_0$ and the $L(E)C_{100}$ are given, the $L(E)C_{50}$ may be estimated.
- 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 test concentration showing no effect. There has to be a concentration-effect relationship.
  In the past, the NOEC was determined directly from the concentration-effect curve by consideration of the deviation of the control (e.g. 10%) or it was derived on the basis of ANOVA (analysis of variance) and a subordinate test (e.g. Dunett's). The preconditions for the use of ANOVA have to be fulfilled (normal distribution, homogeneous variances). This method to derive the NOEC with the ANOVA is criticised (Pack, 1993 (prepared for OECD). The OECD report recommends the calculation of the EC_X point as a preferable alternative (see footnote *). In older investigations, it may be difficult to find out how the NOEC was generated unless test reports or raw data are available.
- A LOEC (lowest observed effect concentration) stands for the lowest concentration where an effect has been observed. It may therefore not be used as a NOEC. In case only a LOEC is given in the report, it can be used to derive a NOEC with the following procedures:
  - LOEC > 10 and < 20% effect: NOEC can be calculated as LOEC/2.
  - LOEC ≥ 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 is often calculated. This is the geometric mean of the NOEC and the LOEC. If in the test report only the MATC is presented, the MATC can be divided by $\sqrt{2}$ to derive a NOEC.
- An 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. This procedure is used if no NOEC is available.
- It should be noted that in the case of algae studies, which are actually multigeneration studies, it is generally accepted that a 72 hour (or longer) EC_{50} value may be considered as equivalent to a short-term result and that a 72 hour (or longer) NOEC value can be considered as a long-term result.

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

3.3 Effects assessment for the aquatic compartment

3.3.1 Calculation of PNEC

The function of risk assessment is the overall protection of the environment. Certain assumptions are made concerning the aquatic environment which allow, however uncertain, an extrapolation to be made from single-species short-term toxicity data to ecosystem effects. It is assumed that:

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

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

For all new substances the pool of data from which to predict ecosystem effects is very limited: only short-term data are available at the base-set. For most existing substances the situation is the same: in many cases, only short-term toxicity data are available. In these circumstances, it is recognised that, while not having a strong scientific validity, empirically derived assessment factors must be used. Assessment factors have also been proposed by the EPA and OECD (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.
  (Extrapolation is required from mono-species tests to ecosystem. Additive, synergistic and antagonistic effects arising from the presence of other substances may also play a role).

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 data-sets than the base-set data. The proposed assessment factors are presented in Table 14.

For new substances an assessment factor of 1000 will be applied on the lowest L(E)C50 of the base-set. Also for existing substances the assessment factor is generally applied to the lowest of the relevant available toxicity data, irrespective of whether the species tested is a standard organism (see notes to Table 14). For short-term tests, the $L(E)C_{50}$ is used, while the NOEC is used with long-term tests. 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 arithmetic mean if more than one $L(E)C_{50}$ value is available for the same species. Prior to calculating the arithmetic mean an analysis of test conditions has to be done in order to find out why differences in response were found.

The algal growth inhibition test of the base-set is, in principle, a multigeneration test. However, for the purposes of applying the appropriate assessment factors, the EC_{50} is treated as a short-term toxicity value. The NOEC from this test may be used as an additional NOEC when other long-term data are available. In general, an algal NOEC should not be used unsupported by long-term NOECs of species of other trophic levels. However, if a chemical shows a specific toxicity to algae, the algal NOEC determined from the base-set test should be supported by a second algae species test.

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

Table 14 *Assessment factors to derive a PNEC*

	Assessment factor
At least one short-term $L(E)C_{50}$ from each of three trophic levels of the base-set (fish, Daphnia and algae)	1000 [(a)]
One long-term NOEC (either fish or Daphnia)	100 [(b)]
Two long-term NOECs from species representing two trophic levels (fish and/or Daphnia and/or algae)	50 [(c)]
Long-term NOECs from at least three species (normally fish, Daphnia and algae) representing three trophic levels	10 [(d)]
Field data or model ecosystems	Reviewed on a case by case basis[(e)]

NOTES:

(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 above identified uncertainties 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 (see section 3.3.2) under no circumstances should a factor lower than 100 be used in deriving a $PNEC_{water}$ from short-term toxicity data.
Evidence for varying 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. (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 raised factor);
- The availability of data from a wide selection of species covering additional taxonomic groups other than those represented by the base-set species;
- The availability of data from a variety of species covering the taxonomic groups of the base-set species across at least three trophic levels.

In such a case the assessment factors may only be lowered if these multiple data points are available for the most sensitive taxonomic group.

There are cases where the base-set is not complete: e.g. for substances which are produced at <1 t/a (notifications according to Annex VII B of Directive 92/32/EEC). At the most the acute toxicity for Daphnia is determined. In these exceptional cases, the PNEC should be calculated with a factor of 1000.
Variation from a factor of 1000 should not be regarded as normal and should be fully supported by accompanying evidence.

(b) An assessment factor of 100 applies to a single long-term NOEC (fish or Daphnia) if this NOEC was generated for the trophic level showing the lowest $L(E)C_{50}$ in the short-term tests.
If the only available long-term NOEC is from a species (standard or non-standard organism) which does not have the lowest $L(E)C_{50}$ 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 available.
An assessment factor of 100 applies also to the lowest of two long-term NOECs covering two trophic levels when such NOECs have not been generated from that showing the lowest $L(E)C_{50}$ of the short-term tests.

(c) An assessment factor of 50 applies to the lowest of two NOECs covering two trophic levels when such NOECs have been generated covering that level showing the lowest $L(E)C_{50}$ in the short-term tests. It also applies to the lowest of three NOECs covering three trophic levels when such NOECs have not been generated from that level showing the lowest $L(E)C_{50}$ in the short-term tests.

(d) An assessment factor of 10 will normally only be applied when long-term toxicity NOECs are available from at least three species across three trophic levels (e.g. fish, Daphnia, and algae or a non-standard organism instead of a standard organism).
When examining the results of long-term toxicity studies, the $PNEC_{water}$ should be calculated from the lowest available no observed effect concentration (NOEC). Extrapolation to the ecosystem effects can be made with much greater confidence, and thus a reduction of the assessment factor to 10 is possible. This is only sufficient, however, if the species tested can be considered to represent one of the more sensitive groups. This would normally only be possible to determine if data were available on at least three species across three trophic levels.

It may sometimes be possible to determine with high probability that the most sensitive species has been examined, i.e. that a further long-term NOEC from a different axonomic group would not be lower than the data already available. In those circumstances, a factor of 10 applied to the lowest NOEC from only two species would also be appropriate. This is particularly important if the substance does not have a potential to bioaccumulate. If it is not possible to make this judgement, then an assessment factor of 50 should be applied to take into account any interspecies variation in sensitivity. A factor of 10 cannot be decreased on the basis of laboratory studies.

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

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

For substances for which no toxicity is observed in short term tests a long term test has to be carried out if the log Kow > 3 (or BCF > 100) and if the $PEC_{local/regional}$ is > 1/100th of the water solubility (see section 4.5). 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 algae test of the base-set an assessment factor of 50 is applied.

The effects assessment performed with assessment factors can be supported by a statistical extrapolation method if the data basis is sufficient for its application (see Appendix V).

3.3.2 Effects assessment for substances with intermittent release

For substances subject to intermittent release (see section 2.3.3.4 for the definition of intermittent release), exposure may be of only short duration. At least for dynamic systems like rivers the likelihood of long-term effects arising from such exposure is low, the principal risk being short-term toxicity effects. In extrapolating to a $PNEC_{water}$, therefore, generally only short-term effects need to be considered. It is therefore proposed that normally an assessment factor of 100 be applied to the lowest $L(E)C_{50}$ of at least three short-term tests from three trophic levels to derive a $PNEC_{water}$ for such situations. The assessment factor is used to allow the extrapolation from the short-term toxicity laboratory test to short-term effects in 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 the aquatic organism which can lead to delayed effects even after emission has stopped. 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 justified.
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 micro-organisms in a STP

As chemicals may cause adverse effects on microbial activity in STPs it is necessary to derive a $PNEC_{micro\text{-}organisms}$ (see section 2.3.7). The $PNEC_{micro\text{-}organisms}$ will be used for the calculation of the PEC/PNEC ratio concerning microbial activity in STPs. Current test systems for measuring the impact of chemicals on microbial activity have different endpoints and sensitivities. At present, only a few internationally accepted test systems, such as OECD 209 (inhibition of respiration of activated sludge) and ISO 9509 (inhibition of nitrification) exist. Available data (e.g. Umweltbundesamt, 1993; Reynolds et al., 1987) suggest the following range of increasing sensitivities: respiration inhibition test (OECD 209) < inhibition control in base-set tests < growth inhibition test with *P. putida* < inhibition of nitrification.
Generally, short-term measurements in terms of hours (e.g. 10 h) are preferred, in accordance with the retention time in a STP. Also the information available on the toxicity for micro-organisms has to be relevant for the endpoint considered, i.e. microbial degradation activity in a STP. It is clear that test systems like the respiration inhibition test and inhibition of nitrification test can be used. Respiration tests using a mixed inoculum are considered more relevant than respiration inhibition tests using another inoculum. Often also information may be present on individual bacterial population like MICROTOX, Pseudomonas putida, Pseudomonas fluorescens and even Escherichia coli. These tests must be considered as less relevant. The tests with P. fluorescens and E. coli (Bringmann and Kühn, 1960) cannot be used for determination of the $PNEC_{micro\text{-}organisms}$ as they use glucose as substrate. Also the MICROTOX test cannot be used as a saltwater species is tested. Results of the cell multiplication inhibition test with P. putida (Bringmann and Kühn, 1980) can be used but should be treated with care.
For assessing the toxicity for a substance to micro-organisms in a STP, the effluent concentration will be compared to microbial effect data. A $PNEC_{micro\text{-}organisms}$ is derived as follows:

- the $PNEC_{micro\text{-}organisms}$ is set equal to a NOEC from a test performed with 'specific bacterial populations' like nitrifying bacteria and *P. putida*. An EC50 from this test is divided by an assessment factor of 10;
- a NOEC or EC10 from other test systems like the respiration inhibition test (OECD 209) is divided by an assessment factor of 10. An EC50 from this test is divided by an assessment factor of 100. It should be noted that the effluent concentration is used while heterotrophic micro-organisms in the aeration tank are probably exposed to a concentration which relates more to the influent concentration. Therefore a higher assessment factor is applied compared to the assessment factor for nitrifying bacteria. For nitrifying bacteria the exposure concentration is more related to the effluent concentration since nitrification is the last treatment step in a STP;
- the lowest value is selected as the $PNEC_{micro\text{-}organisms}$.

3.5 Effects assessment for the sediment

3.5.1 Introduction

Sediments may act as a sink for, and source of chemicals (through resuspension), through sorption of chemical contaminants to particulate matter. 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 in many habitats the sediment plays an important role in the recycling of detrital material.
No data for sediment dwelling organisms will be available for new substances. To date, only few tests for sediment organisms have been conducted in Europe with existing substances. Research is in progress in this field in various countries however. The selection of representative organisms and the selection of standardised sediments are still being discussed. Various approaches (e.g. equilibrium partitioning, interstitial water quality, spiked sediment toxicity, tissue residue, derived sediment quality criteria and standards) are being developed to investigate the effects chemicals have on sediment and sediment organisms (OECD, 1992b). When standardised tests have been conducted and the assessment factors agreed upon, the calculated $PNEC_{sed}$ can be compared with the estimated concentration in the sediment (PEC_{sed}) or with the concentration of the chemical measured in the sediment. Test procedures are described in ASTM (1990 a-e), ASTM (1991) and Burton (1991 and 1992). In addition OECD is preparing a detailed review paper on aquatic ecotoxicity tests including sediment test methods (Water Quality Institute and RIVM, final draft 1995). In Appendix VI sediment toxicity tests are listed which are used in the United States (Burton, 1991).

3.5.2 Calculation of PNEC

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

- Sediment-dwelling organisms and water column organisms are equally sensitive to the chemical;
- Concentration 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).

Based on the equilibrium partitioning the following formula is applied:

$$PNEC_{sed} = \frac{K_{sed\text{-}water}}{RHO_{sed}} \cdot PNEC_{water} \cdot 1000 \qquad (54)$$

Explanation of symbols

$PNEC_{water}$	Predicted No Effect Concentration in water	$[mg.l^{-1}]$	
RHO_{sed}	bulk density of wet sediment	$[kg.m^{-3}]$	eq. (4)
$K_{sed\text{-}water}$	partition coefficient sediment water	$[m^3.m^{-3}]$	eq. (9)
$PNEC_{sed}$	Predicted No Effect Concentration in sediment	$[mg.kg^{-1}]$	

Regardless of whether the $K_{sed\text{-}water}$ is measured or estimated, the following remark has to be made for the calculation of $PNEC_{sed}$ using the equilibrium partitioning method. The formula only considers uptake via the water phase. However, uptake may also occur via ingestion of sediment. This may become important, especially for adsorbing chemicals, for example those with a log Kow greater than 3 (equivalent to a calculated Kp_{sed} of 20 with a Foc of 5%). Thus, for these compounds the total uptake may be underestimated. There is evidence from studies in soil (Belfroid et al., 1995), that the proportion of the total dose remains low for chemicals with a log Kow up to 5. Although it is recognised that in principle results for the soil compartment may not be extrapolated to the sediment compartment, it is considered that the possible underestimation of exposure is acceptable when using the equilibrium partitioning method for chemicals with a log Kow between 3 and 5. For compounds with a log Kow greater than 5 (or with a corresponding Kp_{sed}) the equilibrium method is used in a modified way.

In order to take uptake via ingestion of sediment into account, the PEC_{sed} is increased by a factor of 10 for these compounds. It should be kept in mind that this approach is considered as a screening for assessment of the risk to sediment dwelling organisms. The assessment approach described here should be developed further in the future.

When no measured data on sediment and sediment organisms are available, the assessment conducted on the aquatic compartment will also cover the sediment for chemicals with a log Kow up to 5. If a measured bulk concentration in sediment is available, the formula can be applied and the $PNEC_{sed}$ compared with the measured concentration. This will be the normal situation but other situations may also occur. In Table 15 an overview is given of all possibilities and how to carry out the assessment. The table presents different data configurations and it explains how to use them for the risk characterisation for sediment. If no measured data are available, either for the determination of PEC_{sed} nor for the calculation of $PNEC_{sed}$, no quantitative risk characterisation for sediment can be performed.

Table 15 *Requirements for performing a risk characterisation for sediment*

Available measured data: PEC_{sed}	**Available measured data: $PNEC_{sed}$**	**Risk characterisation**
$C_{pore\ water}$	none	$\frac{C_{pore\ water}}{PNEC_{water}}$
C_{bulk}	none	$\frac{C_{bulk} \cdot RHO_{sed.}}{K_{sed\text{-}water} \cdot PNEC_{water} \bullet \mathbf{1000}}$
none	$PNEC_{sed}$	$\frac{K_{sed\text{-}water} \cdot PEC_{water} \bullet \mathbf{1000}}{PNEC_{sed} \cdot RHO_{sed.}}$
$C_{pore\ water}$	$PNEC_{sed}$	$\frac{K_{sed\text{-}water} \cdot C_{pore\ water} \bullet \mathbf{1000}}{PNEC_{sed} \cdot RHO_{sed.}}$
C_{bulk}	$PNEC_{sed}$	$\frac{C_{bulk}}{PNEC_{sed}}$

where:

$C_{pore\ water}$	concentration in sediment pore water [$mg.l^{-1}$]	
C_{bulk}	concentration in whole sediment [$mg.kg_{sed}^{-1}$]	
$K_{sed\text{-}water}$	sediment-water partitioning coefficient [$m^3.m^{-3}$]	eq. (9)
RHO_{sed}	density of moistened sediment [$kg.m^{-3}$]	eq. (4)

3.6 Effects assessment for the terrestrial compartment

3.6.1 Introduction

Chemicals can reach the soil via several routes: application of sewage sludge in agriculture, direct application of chemicals and deposition from the atmosphere. This means that the possibility of adverse effects has to be assessed. The proposed strategy in this section is based on effects of chemicals on soil organisms. At the moment no strategy is available to assess possible effects on soil functions like 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 can influence soil functions. Substances that are hydrophilic and that are readily eluted with the rain water into the ground water as well as those that geoaccumulate and those that are poorly degradable in soil should be considered with special care.
The terrestrial ecosystem comprises both 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 a provisional one. However, reference is made to the strategy for the compartment air (section 3.7) and for bioaccumulation and secondary poisoning of birds and mammals (section 3.8). So far, it is not possible to carry out effect assessment for the groundwater community because no toxicity data are available. Ecotoxicity tests with groundwater fauna and microflora have been proposed by Notenboom and Boessenkool (1992) and Van Beelen et al. (1990).

The strategy described is based on several documents for terrestrial effects assessment: OECD (1989), Stavola (1990), Pedersen and Samsoe-Petersen (1994), Umweltbundesamt (1993) and Römbke et al. (1993).

3.6.2 Strategy for effects assessment for soil organisms

For most chemicals the number of toxicity data on soil organisms will be limited. At the base-set level for new and existing substances there is no requirement for toxicity tests with soil organisms. For new substances toxicity tests with plants and earthworms can be requested at level 1. At level 2 there are, as yet, no specific additional requirements to examine effects on soil organisms. For existing substances data will probably be scarce: for most chemicals the data set will consist of short term tests for earthworms and plants. Long term tests exist for e.g. micro-organisms, springtails and earthworms but results from these tests are not commonly found for existing substances. Therefore a strategy is proposed to compensate for this lack of toxicity data by using the equilibrium partitioning method conform to the approach for sediment (section 3.5).

Soils used in ecotoxicological tests differ in characteristics like organic matter and clay content, soil pH and soil moisture content. The bioavailability of the test compound, and therefore the toxicity found, is influenced by these soil properties. This means that results from different test soils cannot be compared as such. Subsequently, data have to be normalised using relationships which describe the bioavailability of chemicals in soils. Results are converted to a standard soil, which is defined as a soil with an organic matter content of 3.4% (see section 2.3.4). For non-ionic organic compounds it is assumed that bioavailability is determined by the organic matter content, only. NOECs and $L(E)C_{50}$s are corrected according to the formula:

$$NOEC\ or\ L(E)C_{50(standard)} = NOEC\ or\ L(E)C_{50(exp)} \cdot \frac{Fom_{soil(standard)}}{Fom_{soil(exp)}} \qquad (55)$$

Explanation of symbols

NOEC or $L(E)C50_{exp}$	NOEC or L(E)C50 in experiment	[$mg.kg^{-1}$]	
$Fom_{soil(standard)}$	fraction organic matter in standard soil	[$kg.kg^{-1}$]	Table 3
$Fom_{soil(exp)}$	fraction organic matter in experimental soil	[$kg.kg^{-1}$]	
NOEC or $L(E)C50_{standard}$	NOEC or L(E)C50 in standard soil	[$mg.kg^{-1}$]	

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

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

3.6.2.1 Calculation of PNEC using the equilibrium partitioning method

As for sediment the equilibrium partitioning method for soil assumes that the bioavailability and therefore the toxicity of chemicals to soil organisms is only determined by the concentration in the pore water of the soil. Further effects that chemicals adsorbed to soil particles have on soil organisms by ingestion are not considered by this approach. The $PNEC_{soil}$ is calculated as follows:

$$PNEC_{soil} = \frac{K_{soil-water}}{RHO_{soil}} \cdot PNEC_{water} \cdot 1000 \qquad (56)$$

Explanation of symbols

$PNEC_{water}$	Predicted No Effect Concentration in water	[mg.l^{-1}]	
RHO_{soil}	bulk density of wet soil	[kg.m^{-3}]	eq. (4)
$K_{soil-water}$	partition coefficient soil water	[m^3.m^{-3}]	eq. (9)
$PNEC_{soil}$	Predicted No Effect Concentration in soil	[mg.kg^{-1}]	

The applicability of the equilibrium partitioning method has been tested 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. As for sediment the equilibrium partitioning method may not be suitable for lipophilic compounds and species that are exposed primarily through food (Van Gestel, 1992). Therefore the same approach is used as for the derivation of the $PNEC_{sediment}$: in order to take uptake via ingestion of soil into account the PEC_{soil} is increased by a factor of 10 for compounds with a log Kow > 5.

In principle, toxicity data for aquatic organisms cannot replace data for soil dwelling organisms, because the effects on aquatic species can only be considered as effects on soil organisms which are exposed exclusively to the pore water of the soil (Pedersen and Samsoe-Petersen, 1993). Therefore if the ratio $PEC_{soil}/PNEC_{soil}$ calculated via the equilibrium partitioning method is greater than 1, tests with soil organisms are indispensable for effects assessment for the soil compartment.

3.6.2.2 Calculation of PNEC using assessment factors

The same assessment factors are used for the terrestrial system (see Table 16) as for the aquatic system (see Table 14) depending on the type of investigations (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 suggested assessment factors for the soil compartment are not based on comprehensive experience. As already stated information from tests with soil organisms will only be available for some compounds. Also, in most cases this will be information from short-term tests with earthworms. This means that a deeper understanding of the difference between short- and long-term toxicity for several taxonomic groups and the difference between laboratory and field tests is needed. Also the choice of taxonomic groups for which toxicity data are necessary (conform the base-set of algae, Daphnia and fish for the aquatic environment), is a point of discussion. A data-set consisting of toxicity data for primary producers, consumers and decomposers is preferred. However, an internationally accepted set of standardised ecotoxicological tests for hazard assessment of chemicals for the soil compartment is not available at the moment.

Reference can be made to section 5.2.3 and an OECD project in which a testing strategy for terrestrial ecosystems is being developed (Léon and Van Gestel, 1994). Summarising, the assessment factors proposed in Table 16 must be regarded as indicative factors. As more information on the sensitivity of soil organisms becomes available these factors may have to be adjusted.

Table 16 *Assessment factors to derive a PNEC*

Information available	Assessment factor
$L(E)C_{50}$ short-term toxicity tests (e.g. plants, earthworms, or micro-organisms)	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
Field data/data of model ecosystems	case-by-case

The $PNEC_{soil}$ is calculated on the basis of the lowest effect value measured. If short-term tests with a producer, a consumer and/or a decomposer are available, the test result is divided by a factor of 1000 to calculate the $PNEC_{soil}$. If only one terrestrial test is available (earthworms or plants), the risk assessment should be performed both on the basis of this terrestrial test and on the basis of the aquatic toxicity data as an indication of the risk to soil organisms. As a precaution, the larger PEC_{soil} /$PNEC_{soil}$ ratio determines which further actions should be taken in the framework of the further testing strategy. The other factors listed in Table 16 are applied, if more tests than the short-term toxicity test have been conducted.

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 clear 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 for new and existing substances. 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 new nor for existing substances. For some existing substances investigations on the toxicity of 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, there are almost no data available from tests where a chemical is applied directly via air (gaseous or deposited). Tests with herbaceous species would be desirable but are performed in only a few cases. A guideline for these tests has not been accepted yet.

3.7.2 Abiotic effects

For the evaluation of an atmospheric risk, the following abiotic effects of a chemical on the atmosphere have to be considered:

- global warming;
- ozone depletion in the stratosphere;
- ozone formation in the troposphere;
- acidification.

If for a chemical there are indications that one or several of these effects occur, expert knowledge should be consulted. A first quantitative approach is described in De Leeuw (1993):

Global warming

The impact of a substance on global warming depends on its IR absorption characteristics and its atmospheric lifetime. A potential greenhouse gas shows absorption bands in the so-called atmospheric window (800-1200 nm).

Stratospheric ozone

A substance may have an effect on stratospheric ozone if e.g.

- the atmospheric lifetime is long enough to allow for transport to the stratosphere, and;
- it contains one or more Cl or Br 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 have to exceed several ppb.

Highly reactive compounds (e.g. xylene, olefins or aldehydes) contribute significantly to the ozone peak values. Species with a low reactivity (e.g. CO, methane) are important for ozone formation in the free troposphere and therefore for the long-term ozone concentrations. However, all studies showed significant variability in the tropospheric ozone building potential values assigned to each organic component. It has to be concluded that at present there is no procedure available to estimate the effect on tropospheric ozone if only the basic characteristics of a substance are known.

Acidification

During the oxidation of substances containing Cl, F, N or S substituents, acidifying components (e.g. HCl, HF, NO_2 and HNO_3, SO_2 and H_2SO_4) may be formed. After deposition, these oxidation products will lead to acidification of the receiving soil or surface water.

3.8 Assessment of secondary poisoning

3.8.1 Introduction

Bioconcentration and bioaccumulation may be of concern for lipophilic organic chemicals and some metal compounds as both direct and indirect toxic effects may be observed upon long term exposure. For metals guidance is given in Appendix VIII. Bioconcentration is defined as the net result of the uptake, distribution and elimination of a substance in an organism due to water-borne exposure, whereas bioaccumulation includes all routes, i.e. air, water, soil and food. Biomagnification is defined as accumulation and transfer of chemicals via the food chain, resulting in an increase of the internal concentration in organisms at higher levels in the trophic chain. Secondary poisoning is concerned with toxic effects in the higher members of the food chain, either living in the aquatic or terrestrial environment, which result from ingestion of organisms at the different trophic levels that contain accumulated substances.

For many hydrophobic chemicals accumulation through the food chain follows many different pathways along different trophic levels. A good risk estimation of this complex process is hampered when only limited data from laboratory studies are available. One way to assess a chemicals risk for bioaccumulation in aquatic species is to measure the Bioconcentration Factor (BCF). The static bioconcentration factor is the ratio between the concentration in the organism and the concentration in water in a steady-state (sometimes also called equilibrium) situation. When uptake and depuration kinetics are measured, the dynamic bioconcentration factor can be calculated from the quotient of the uptake and depuration rate constants:

$$BCF_{fish} = \frac{C_{fish}}{C_{water}} \quad or \quad \frac{k_1}{k_2} \tag{57}$$

Explanation of symbols

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

For new and existing substances, the assessment of these processes is revised as more information becomes available on toxicological and ecotoxicological effects and exposure. At the base-set level the available physico-chemical and (eco)toxicological information can be used to decide whether or not there are indications for a potential for bioaccumulation and/or indirect effects. This estimation is used as a first step in the testing strategy for bioaccumulation and secondary poisoning as will be explained in section 3.3.8. For the terrestrial ecosystem a similar strategy is used which is described in section 3.3.8.

3.8.2 Indication of bioaccumulation potential

The simplest way to estimate the potential of a substance to bioaccumulate in aquatic species is by experimental measurement of the BCF. Determination of the BCF alone, however, only gives a partial picture of the potential of bioaccumulation, and additional data on uptake and depuration kinetics, metabolism, organ specific accumulation and the level of bound residues may also be required. Such data will rarely be available and the potential for bioaccumulation will usually need to be determined using simple physico-chemical and structural evidence.
The most important and widely accepted indication of bioaccumulation potential is a high value of the n-octanol/water partition coefficient. In addition, if a substance belongs to a class of chemicals which are known to accumulate in living organisms, it may have a potential to bioaccumulate. However, some properties of a substance may preclude high accumulation levels even though the substance has a high log Kow or has a structural similarity to other substances likely to bioaccumulate. Alternatively there are properties which may indicate a higher bioaccumulation potential than that suggested by a substance's low log Kow value. A survey of these factors is given below.

n-Octanol/Water Partition Coefficient
At the base-set level, the potential for bioaccumulation can be estimated from the value of the n-octanol/water partition coefficient, log Kow. If this value cannot be determined experimentally, it may be calculated from the chemical structure.

It is accepted that values of log Kow greater than or equal to 3 indicate that the substance may bioaccumulate. For certain types of chemicals, e.g. surface-active agents and those which ionise in water, log Kow values may not be suitable for calculation of a BCF value. There are, however, a number of factors that are not taken into consideration when BCF is estimated only on the basis of log Kow values. These are:

- phenomena of active transport;
- changes in the behaviour of diffusion through cell membranes;
- metabolism in organisms and the accumulation potential of any metabolites;
- affinity due to specific interactions with tissue components;
- special structural properties (e.g. amphiphilic substances or dissociating substances that may lead to multiple equilibrium processes);
- uptake and depuration kinetics (leading for instance to a remaining concentration plateau in the organism after depuration).

n-Octanol only simulates the lipid fraction in organisms and therefore does not simulate other possibilities for storage and accumulation of substances and their metabolites in living organisms.

Adsorption

Adsorption onto biological surfaces, such as gills or skin, may also lead to bioaccumulation and an uptake via the food chain. Hence, high adsorptive properties may indicate a potential for both bioaccumulation and biomagnification. For certain chemicals, for which the octanol/water partition coefficient cannot be measured properly, a high adsorptive capacity (of which log Kp > 3 may be an indication) can be additional evidence of bioaccumulation potential.

Hydrolysis

The effect of hydrolysis may be a significant factor for substances discharged mainly to the aquatic environment: the concentration of a substance in water is reduced by hydrolysis so the extent of bioconcentration in aquatic organisms would also be reduced. Where the half life, at environmentally relevant pH values (4-9) and temperature, is less than 12 hours, it can be assumed that the rate of hydrolysis is greater than that for uptake by the exposed organisms. Hence, the likelihood of bioaccumulation is greatly reduced. In these cases, it may sometimes be appropriate to perform a BCF test on the hydrolysis products, if identified, instead of the parent substance. However, it should be noted that, in most cases hydrolysis products are more hydrophilic and as a consequence will have a lower potential for bioaccumulation.

Degradation

Both biotic and abiotic degradation may lead to relatively low concentrations of a substance in the aquatic environment and thus to low concentrations in aquatic organisms. However, the uptake rate may still be greater than the rate of the degradation processes, leading to high BCF values even for readily biodegradable substances. Therefore ready biodegradability does not preclude a bioaccumulation potential, but for most substances concentrations will be low in aquatic organisms.

At the base-set level, only scarce information on the kinetics of degradation is available. For new substances even at higher tonnages, a request for such information would need to be justified; it can be requested only on a case-by-case basis at level 2. For existing substances information on degradation kinetics may be available.

If persistent metabolites are formed in substantial amounts the bioaccumulation potential of these substances should also be assessed. However, for most substances information will be scarce. From experiments with mammals information may be obtained on the formation of possible metabolites, although extrapolation of results should be treated with care.

Molecular Mass

Certain classes of substances with a molecular mass greater than 700 are not readily taken up by fish, mainly because of possible steric hindrance at passage of cell membranes. These substances are unlikely to bioaccumulate significantly (regardless of the log Kow-value).

Summary of Indications of Bioaccumulation Potential

Taking the factors mentioned above into account will indicate whether or not there is potential for bioaccumulation. Criteria based on these factors are summarised below.

Positive indications: if, at base-set level, a substance

- has a log Kow ≥ 3; or;
- is highly adsorptive; or;
- belongs to a class of substances known to have a potential to accumulate in living organisms; or;
- there are indications from structural features;
- and there is no mitigating property such as hydrolysis (half life less than 12 hours);

there is an indication of bioaccumulation potential.

3.8.3 Effects assessment for bioaccumulation and secondary poisoning

3.8.3.1 General approach

A strategy for the assessment of the occurrence of secondary poisoning has been developed further to support the decision when to request a bioaccumulation test. This strategy takes account of the PEC_{water}, the resulting concentration in food of higher organisms and the mammalian toxicity of the chemical as an indication of possible effects on birds and mammals in the environment via the food-chain water → fish → fish-eating mammal or fish-eating bird (Romijn et al., 1993). Due to the lack of experience with this approach the assessment is considered as provisional.

For some chemicals results from field measurements are available. Although interpretation is often difficult these results can be used to assess risks due to secondary poisoning (Ma, 1994).

A schematic view of the assessment scheme for the route water → fish → fish-eating mammal or fish-eating bird described above is given in Figure 12. The first step in the scheme 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 certain classifications on the basis of its 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.

If a substance is classified accordingly or if there are other indications, an assessment of secondary poisoning is performed.

At this stage a simple estimation is made if the PEC in water can lead to concentrations in fish that may lead to deleterious effects in higher organisms that eat fish. If secondary poisoning is to be avoided, the concentration of chemicals in the food should be below the No Observed Effect Level (NOEL) in dietary toxicity test with animals representative for fish-eating birds or mammals. The NOEL is considered as a maximum concentration in food which will not lead to adverse effects after ingestion of this food ($PNEC_{oral,fish}$). When the BCF of a substance is known, the PEC_{water} can be used to calculate the PEC in food (PEC_{oral}). This concentration can then be compared with $PNEC_{oral,fish}$.
If no measured BCF, as will normally be the case for new substances, an estimated BCF value based on the octanol/water partition coefficient is used. The decision to request a bioaccumulation test is based on the quantitative outcome of the assessment. A more detailed description of the assessment is given in the sections below.

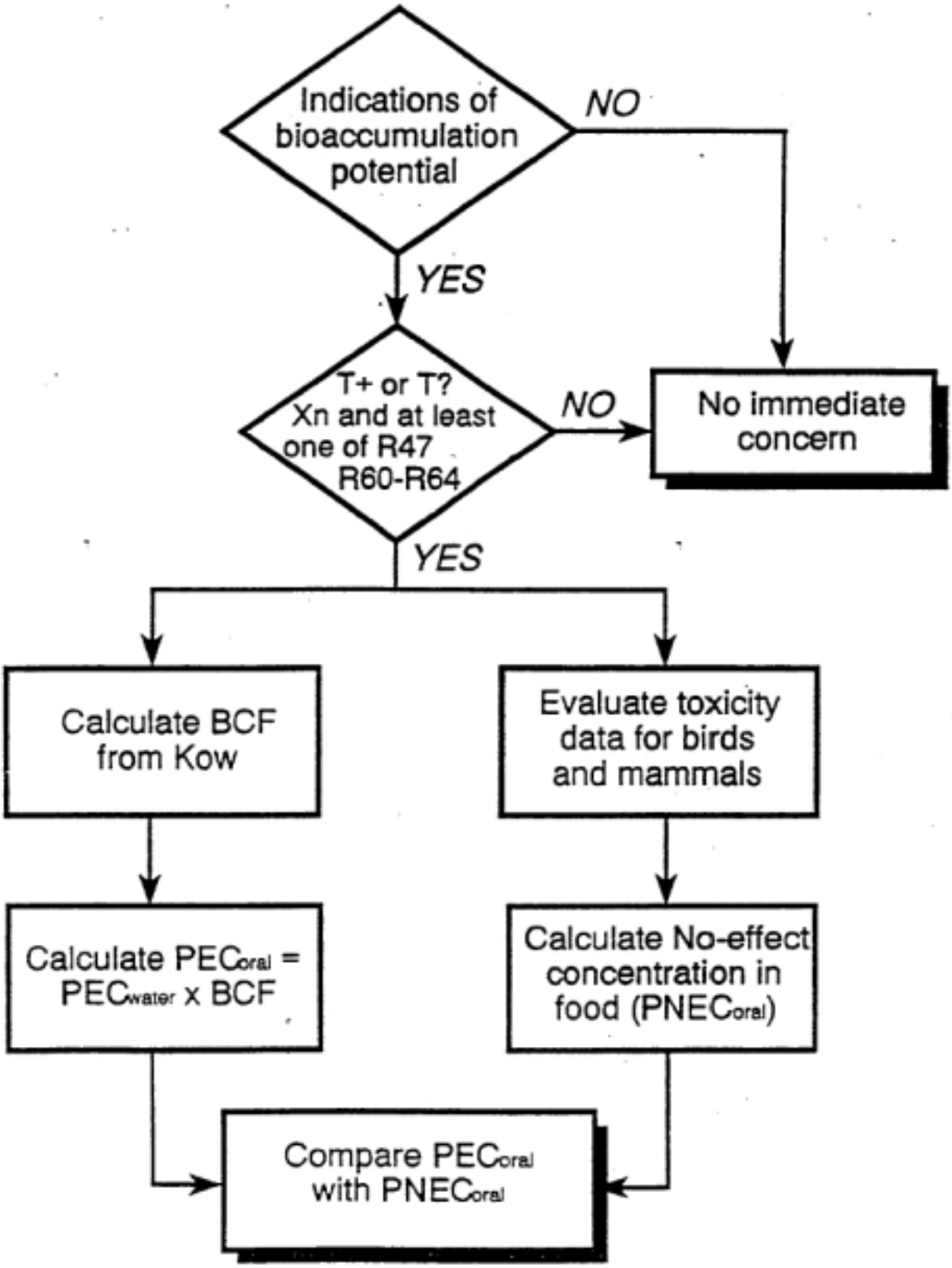

Figure 12 *Assessment scheme for secondary poisoning*

3.8.3.2 Calculation of BCF from log Kow

If measured BCF-values are not available the BCF for fish can be predicted from the relationship between Kow and BCF. Various methods are available to calculate Kow. Often a large variation is found in the Kow-values of a chemical by using different methods. Therefore the Kow-value must have been evaluated by an expert (see also Chapter 4 on the use of QSARs). For substances with a log Kow of 2-6 the following linear relationship can be used as developed by Veith et al. (1979).

$$\log BCF_{fish} = 0.85 \cdot \log Kow - 0.70 \quad (58)$$

Explanation of symbols

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

For substances with a log Kow higher than 6 a parabolic equatic can be used.

$$\log BCF_{fish} = -0.20 \cdot logKow^2 + 2.74 \cdot \log Kow - 4.72 \quad (59)$$

Explanation of symbols

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

Both relationships apply to compounds with a MW less than 700. 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. For a discussion on both relationships see Chapter 4 (Use of QSARs).

3.8.3.3 Experimentally derived BCF

For existing substances an experimentally derived BCF may be present. For new substances a BCF test is mandatory at level 1. In most cases preference should be given to experimentally determined BCF values, especially if the test is conducted according to OECD Guideline 305 E (last revised version) (OECD, 1994). 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.

Recent work has shown that tests with substances with a high log Kow value result in high bioaccumulation factors if the chemical is carefully tested within the limit of its water solubility, i.e. without enhancement of solubility by the use of solubilisers. Also, the test duration is very important because for highly hydrophobic chemicals it may take a very long time before a true steady-state situation between water and organism has been reached. In addition, such lipophilic substances may be adsorbed onto biological surfaces such as gills, skin etc. which may lead to toxic effects in higher organisms after biomagnification.

3.8.3.4 Evaluation of toxicity data for birds and mammals

Only toxicity studies reporting on dietary and oral exposure are relevant as the pathway for secondary poisoning is referring exclusively to the uptake through the food chain. The results of these test may be expressed as a concentration in the food (mg/kg) or a dose (mg/kg body weight/day) causing no effect. For the assessment of secondary poisoning, the results are converted to the concentration in food (mg/kg food). Conversion factors are given in Appendix VII.
Effects on birds and mammal populations are rarely caused by mortality after short-term exposure. Therefore, results from long-term studies are 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.

3.8.3.5 Calculation of the predicted no-effect concentration ($PNEC_{oral}$)

For new substances the results of mammalian repeated dose toxicity test(s) are used in the assessment of secondary poisoning effects.
For existing substances also toxicity data for birds may be present. Extrapolation from such test results can give a predicted no-effect concentration in food that should be protective of other mammalian and avian species. Assessment factors are to be used which take into account interspecies variation, subchronic to chronic toxicity extrapolation and laboratory data to field impact extrapolation.

Acute lethal doses LD_{50} (rat, bird) are not acceptable for extrapolation to chronic toxicity as these tests are not dietary tests. Acute effect concentrations (LC_{50} (5 days) avian dietary studies) are acceptable for birds for extrapolation because for most compounds these are generally the only data available for these vertebrates. An assessment factor of 1,000 can be applied on results from such a test. An assessment factor of 100 (10x10) can be applied to the NOEC for the 28 day repeated dose test to derive the $PNEC_{oral}$. Where a 90-day toxicity text is submitted instead of the 28- day test, this assessment factor may be reduced to 30 (see e.g. EC (1993)).

When chronic studies are available, an assessment factor of 10 may be used. Reproduction toxic effects are regarded as chronic effects and the same assessment factor may be used.

3.8.3.6 Calculation of a predicted environmental concentration in food

The level in food (fish) is calculated from the PEC for surface water and the measured or estimated BCF for fish:

$$PEC_{oral,\ fish} = PEC_{water} \cdot BCF_{fish} \qquad (60)$$

Explanation of symbols

BCF_{fish}	bioconcentration factor for fish on wet weight basis	$[l.kg_{wet\ fish}^{-1}]$
PEC_{water}	Predicted Environmental Concentration in water	$[mg.l^{-1}]$
$PEC_{oral,\ fish}$	Predicted Environmental Concentration in food	$[mg.kg_{wet\ fish}^{-1}]$

There are difficulties in deciding whether the regional or local PEC_{water} must be used for the risk characterisation. Using PEC_{local} may lead to an overestimation of the risk as fish-eating birds or mammals do also fourage 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.
A solution could be to define a new area based on the fouraging range of fish-eating birds and mammals. Another option is to assume that a certain percentage of the diet of fish-eating birds and mammals comes from a source using PEC_{local}, while another percentage comes from a source using $PEC_{regional}$.
Considering that the fouraging range can vary enormously, which makes it difficult to decide on the appropriate scale, the last option is used where 50% of the diet comes from a source using PEC_{local} and 50% using $PEC_{regional}$.
When the predicted concentration in food exceeds the predicted no-effect concentration in food, secondary poisoning can be a critical pathway for fish-eaters. In that case, the provisional assessment of secondary poisoning may lead to testing of the bioconcentration factor in fish so as to facilitate a better assessment of the risk of secondary poisoning. This is discussed in sections 4.3 and 4.4 for existing and new substances, respectively.

3.8.3.7 Assessment of secondary poisoning

The water → fish → fish-eating bird or mammal food chain is 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 the 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 EPA uses a species sensitivity factor (SSF) which ranges from 1 to 0.01.

Whether these factors should be used is still under debate at the moment.

3.8.3.8 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). The PEC_{oral} is calculated as:

$$PEC_{oral,\ worm} = PEC_{soil} \cdot BCF_{earthworm} \qquad (61)$$

Explanation of symbols

$BCF_{earthworm}$	bioconcentration factor for earthworms on wet weight basis	[$kg.kg_{wet\ earthworm}^{-1}$]
PEC_{soil}	Predicted Environmental Concentration in soil	[$mg.kg^{-1}$]
$PEC_{oral,\ worm}$	Predicted Environmental Concentration in food	[$mg.kg_{wet\ earthworm}^{-1}$]

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). The same scenario is used as for the aquatic food chain (see section 2.3.8.6): i.e. 50% of the diet comes from PEC_{local} and 50% from $PEC_{regional}$. Due to the lack of experience with this approach the assessment is considered as provisional.

The $BCF_{earthworm}$ is defined as follows:

$$BCF_{earthworm} = \frac{C_{earthworm}}{C_{soil}} = K_{earthworm\text{-}porewater} \cdot \frac{RHO_{soil} \cdot 10^{-3}}{K_{soil\text{-}water}} \qquad (62)$$

Explanation of symbols

$BCF_{earthworm}$	bioconcentration factor for earthworms on wet weight basis	[$kg.kg_{wet\ earthworm}^{-1}$]	
$C_{earthworm}$	concentration in earthworm	[$mg.kg^{-1}$]	
C_{soil}	concentration in soil	[$mg.kg^{-1}$]	
$K_{earthworm\text{-}porewater}$	partition coefficient earthworm-porewater	[$l.kg_{wet\ earthworm}^{-3}$]	
$K_{soil\text{-}water}$	partitioning coefficient soil-water	[$m^3.m^{-3}$]	eq. (9)
RHO_{soil}	bulk density of wet soil	[$kg.m^{-3}$]	eq. (4)

The BCFs for earthworms is estimated using a QSAR from Connell and Markwell (1990). They derived an empirical equation for $K_{earthworm\text{-}porewater}$ through regression on experimental data for pesticides with a log Kow ranging from 1.0 to 6.5.

$$K_{worm\text{-}porewater} = 0.25 \cdot Kow \qquad (63)$$

Explanation of symbols

$K_{earthworm\text{-}porewater}$	partition coefficient earthworm-porewater	[$l.kg_{wet\ earthworm}^{-1}$]
Kow	partition coefficient n-octanol-water	[-]

As data from experiments conducted under different conditions are included it has to be stated that the sources of variation in this study are substantial. Romijn et al. (1994) showed that for dieldin, DDT and pentachlorophenol geometric mean $BCF_{earthworm}$s obtained from laboratory tests are < 1. These $BCF_{earthworm}$ values were in good agreement with the results reported by Connell and Markwell (1990).

If the predicted concentration in food (PEC_{oral}) exceeds the PNEC, secondary poisoning can be a critical pathway for worm-eating predators. In principle the same approach can be used as for the aquatic route. However, no international accepted guidelines are available at the moment for deriving BCFs for earthworms. Also, for organic compounds this may not be the critical factor here as for most compounds the BCF is close to 1, which can also be concluded from the formula given above (as Koc = 0.411 · Kow). Therefore, it seems more appropriate to refine the PEC for soil, before a test for determination of the $BCF_{earthworm}$ or an additional toxicity test with a mammal or bird is carried out.

4. Risk characterisation

4.1 Introduction

Having conducted the exposure assessment and the dose (concentration) - response (effect) assessment for all environmental compartments, the risk characterisation is carried out by comparing the PEC with the PNEC. This is done separately for each of the protection goals identified in section 1.2 and Table 1:

- aquatic ecosystem;
- terrestrial ecosystem;
- atmosphere;
- top predators;
- micro-organisms in sewage treatment plants.

A list of the different PEC/PNEC ratio's that may follow out of the previous chapters is given in Table 17. Depending on whether the risk characterisation is performed for a new substance or for an existing substance different conclusions can be drawn on the basis of the PEC/PNEC ratio for the different endpoints and different strategies can be followed when PEC/PNEC ratio's greater than one are observed. Therefore in the following sections the risk characterisation for new substances and for existing substances are treated separately. However, a number of general premises apply to the procedures that have to be followed for both new and existing substances. These are given first.

Table 17 *Overview of possible PEC/PNEC ratio's in environmental risk assessment**

Local	**Regional**
$PEClocal_{water}/PNEC_{water}$	$PECregional_{water}/PNEC_{water}$
$PEClocal_{sediment}/PNEC_{sediment}$	$PECregional_{sediment}/PNEC_{sediment}$
$PEClocal_{soil}/PNEC_{soil}$	$PECregional_{agr.soil}/PNEC_{soil}$
$PEC_{STP}/PNEC_{micro\text{-}organisms}$	
$(0.5 \cdot PEClocal_{oral,fish} + 0.5 \cdot PECregional_{oral,fish})/PNEC_{oral}$	
$(0.5 \cdot PEClocal_{oral,worm} + 0.5 \cdot PECregional_{oral,worm})/PNEC_{oral}$	

- It has to be noted that these ratio's have to be derived for all stages of the life-cycle of a compound.

4.2 General premises for risk characterisation

In general, the risk characterisation phase is carried out along the following steps (see Figure 13):

- determining the PEC/PNEC ratio's for the different protection goals.

Dependent on these PEC/PNEC ratio:

- determining whether further information/testing may lead to a revision of these ratio's;
- asking for further information/testing when appropriate;
- refinement of the PEC/PNEC ratio.

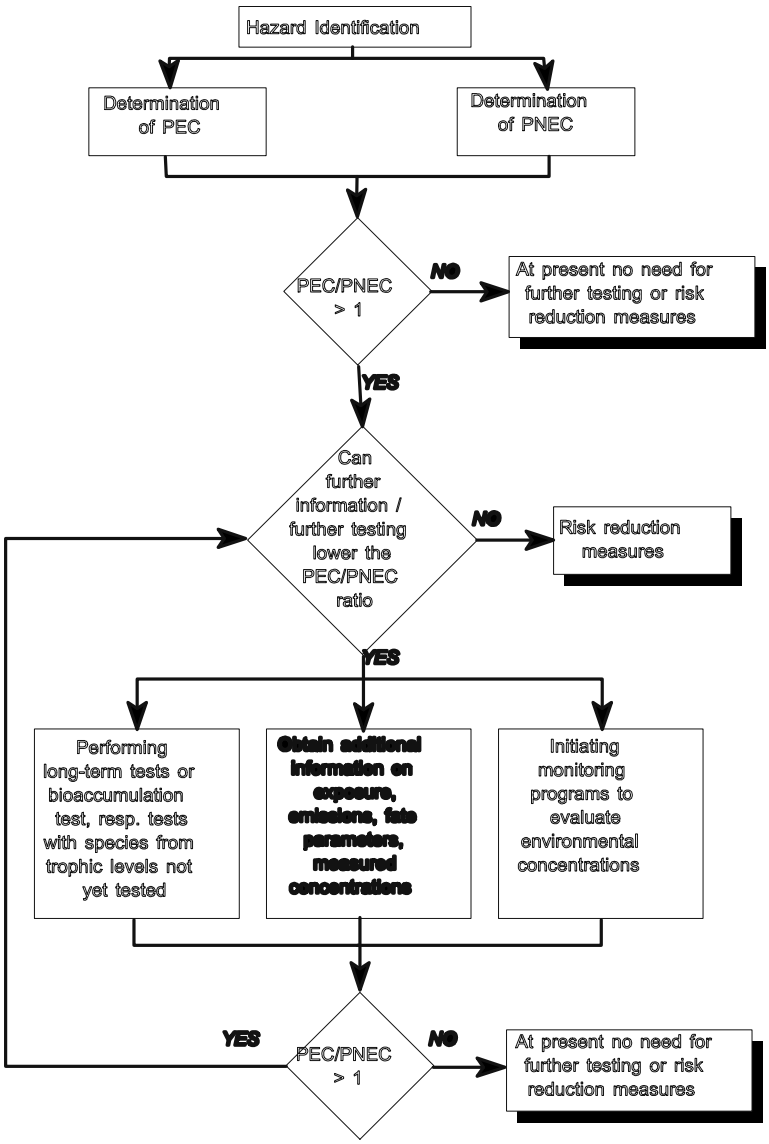

Figure 13 *General procedure for environmental risk assessment of new and existing substances*

This iterative process is continued until one of the following conclusions can be drawn:

- at present there is no need for further testing or risk reduction measures;
- risk reduction measures are necessary.

For the risk characterisation of the aquatic and terrestrial ecosystems 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 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.
The risk characterisation for top predators is made by comparing the PEC_{oral} with the $PNEC_{oral}$ in accordance with the procedure described in section 3.8 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 micro-organisms in sewage treatment systems is done by comparing the PEC_{STP} with the $PNEC_{micro\text{-}organisms}$. 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 ratio's 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.

Subsequently it is decided whether further information/testing may lead to a revision of the PEC/PNEC ratio's. 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, the substance in question should be a candidate for risk reduction and the results of any further testing will not affect that decision.
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 will be more sensitive to revision as a result of further testing. The decision by the competent authority to request the generation of 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.

It also saves resources and takes animal welfare into account as only a minimum of tests has to be performed. Guidance on which tests to conduct and how the results of such tests can be used to revise the PEC and/or the PNEC is given in sections 5.1 and 5.2 of this document. Detailed guidance on how to use (Q)SARs in order to clarify whether further testing is necessary, and how these (Q)SARs can assist in deciding in the testing strategy, is given in Chapter 4 (Use of QSARs).

4.3 Risk characterisation for existing substances

The environmental risk assessment in the context of article 5 and Annex 3 of Regulation 1488/94 involves the comparison of the PEC and PNEC values for the different endpoints mentioned above. Regulation 793/93 mentions three different conclusions that may apply on the basis of the risk characterisation:

(i) there is need for further information and/or testing;
(ii) there is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already;
(iii) there is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

The general scheme given in Figure 13 applies for the risk characterisation of existing substances. At the first comparison of the PEC and PNEC values it is assumed that industry is contacted and that all available information is used to derive these. If the PEC/PNEC ratio is found to be less or equal to one for each compartment, conclusion (ii) shall apply. If the PEC/PNEC ratio is greater than one, the rapporteur shall judge whether further information and/or testing are required to clarify the concern (conclusion (i)) or if risk reduction measures are necessary (conclusion (iii)). The judgement shall be carried out on the basis of the size of the PEC/PNEC ratio and some additional indicators such as:

(i) indications of bioaccumulation potential;
(ii) the shape of the toxicity/time curve in ecotoxicity testing;
(iii) indications of other adverse effects on the basis of toxicity studies, e.g. classification as a mutagen, toxic or very toxic or as harmful with a risk phrase R40 ('Possible risk of irreversible effects') or R48 ('Danger of serious damage to health by prolonged exposure');
(iv) data on structurally analogous substances.

Furthermore indications of other adverse effects, e.g. classification with the risk phrases R45 ('may cause cancer'), R46 ('may cause heritable genetic damage'), R47 ('may cause birth defects') and R60 ('may impair fertility') may be considered as well.

These factors especially pertain to substances for which a "standard" risk assessment cannot be performed, for instance because the models that are applied are not suitable, or for substances which the standard data set does not give the right information on the properties of the substance (for instance highly hydrophobic substances that do not show any toxicity in short term tests).

A specific risk characterisation is made for secondary poisoning. PEC_{oral} and $PNEC_{oral}$ are calculated according to the procedures described in section 3.8, either by using the available BCF values or by calculation of BCF from the octanol/water partition coefficient. Both the local and the regional PEC_{water} are used (50/50) to calculate PEC_{oral}.

4.4 Risk characterisation for new substances

The risk characterisation in the context of article 5 of and Annex III to Directive 93/67/EEC also involves the iterative revision of the PEC/PNEC ratio as a function of the degree of risk predicted. In addition, a link is made with the tonnage triggers for further testing as laid down in Article 7.2 of Directive 67/548/EEC. If the PEC/PNEC ratio is found to be less than or equal to one, the conclusion laid down in Article 3. 4(i) of the Directive shall apply:

- the substance is of no immediate concern and need not to be considered again until further information is made available in accordance with Articles 7(2), 8(3), 8(4) or 14(1) of the parent Directive 67/548/EEC.

If the PEC/PNEC ratio is greater than one the authority should judge which of the conclusions set out in Article 3.4(ii), 3.4(iii) or 3.4(iv) shall apply:

- the substance is of concern and the competent authorities shall decide what further information is required for revision of the assessment but shall defer a request for that information until the quantity placed on the market reaches the next tonnage threshold as indicated in Article 7(2), 8(3) or 8(4) of Directive 67/548/EEC;
- the substance is of concern and further information shall be requested immediately;
- the substance is of concern and the competent authority shall immediately make recommendations for risk reduction.

In the light of rather extensive experience of testing and evaluation procedures linked with the aquatic environment, it has been possible to develop a relatively structured decision scheme in relation to the aquatic compartment. This scheme is given in Figure 14.

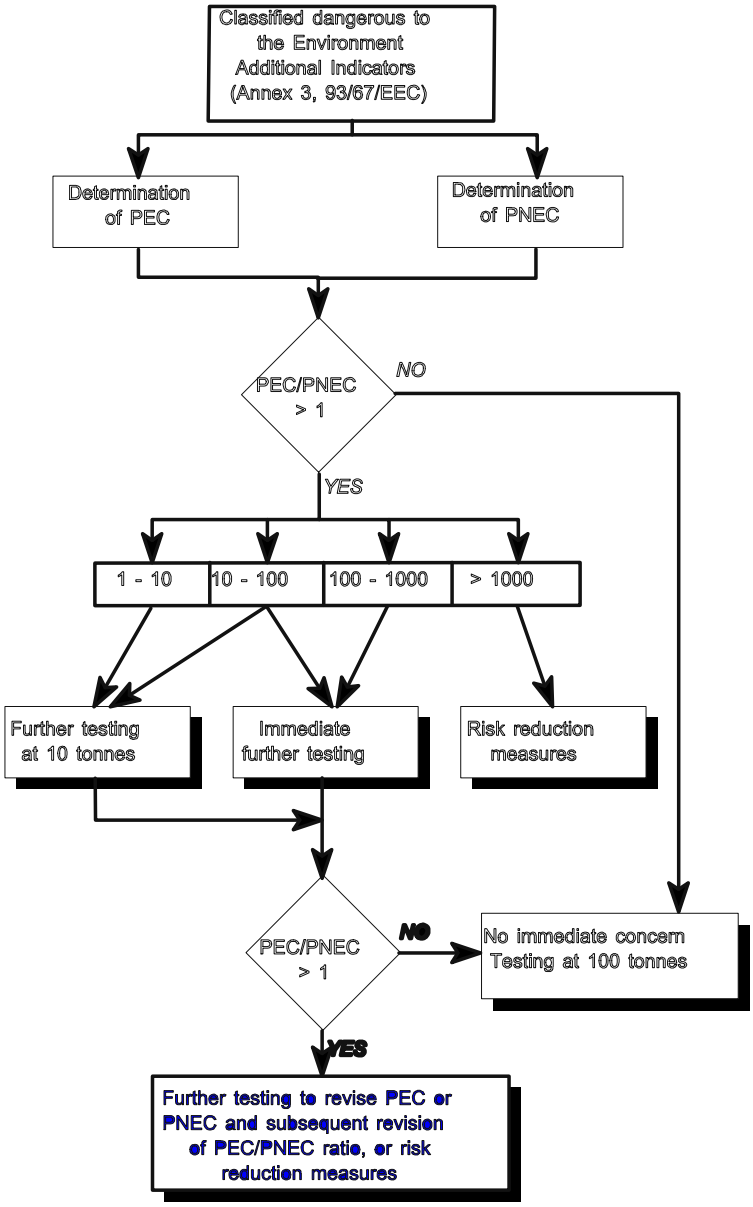

Figure 14 *Decision scheme for aquatic risk characterisation of new chemicals*

It is assumed that for substances entering the scheme, data equivalent to those foreseen in Annex VII A (the base set) to Directive 67/548/EEC will be available. Information contained in the base set is used to estimate the PEC and the PNEC for the aquatic environment. Furthermore the assumption is made in the decision scheme that where the PEC/PNEC ratio exceeds one, the authority has discussed this situation with the notifier and that the values, in particular the PEC, have already been amended in the light of further information provided by the notifier. The first PEC/PNEC ratio referred to in Figure 14 is therefore the value as amended after further discussions with the notifier.

Depending on the value of the PEC/PNEC ratio, one of the options available under article 3.4 of Directive 93/67/EEC is chosen. Where the PEC/PNEC ratio is between 10 and 100, the decision whether to request further testing immediately or at the 10 tonnes per annum production level will be made on the basis of a number of factors including:

(i) indications of bioaccumulation potential;
(ii) the shape of the toxicity/time curve in ecotoxicity testing;
(iii) data on structurally analogous substances.

The factor "indications of other adverse effects on the basis of toxicity studies, e.g. classification as a mutagen, as toxic or very toxic or as harmful with risk phrase R40 ('possible risk of irreversible effects') or R48 ('danger of serious damage to health by prolonged exposure')" can be used to decide whether a substance will enter the scheme; so whether a risk assessment should be performed. This factor cannot be used to decide whether further testing is needed.

The base set testing package (Annex VII A) of the Directive generates relatively little data which are of relevance to the terrestrial and atmospheric compartments: further but nevertheless limited data are foreseen at level 1 and level 2 (Annex VIII). Where consideration of either of these two compartments is of relevance to the environmental risk assessment of a particular substance, further testing and progressive revision of the PEC/PNEC should be carried out on a case-by-case basis in the light of the guidance set out in section 5. For the risk characterisation for top predators a specific assessment scheme applies. This scheme is given in Figure 15. In this case the yearly-average PEC_{local} for water is used to calculate PEC_{oral}. Based on the results of the provisional assessment of secondary poisoning where a calculated BCF value is used (see section 3.8), it is decided whether or not a BCF test should be requested, either immediately or at the 10 tonnes per annum production level. It should be noted that an BCF test is a level 1 test. The result of the BCF test is used to refine the risk characterisation for top predators. If the ratio of PEC_{oral} and $PNEC_{oral}$ is still greater than one, secondary poisoning could be a critical pathway for fish eaters. This may lead to a request for more specific tests, for instance long-term dietary studies on birds, that can be used to facilitate a better calculation.

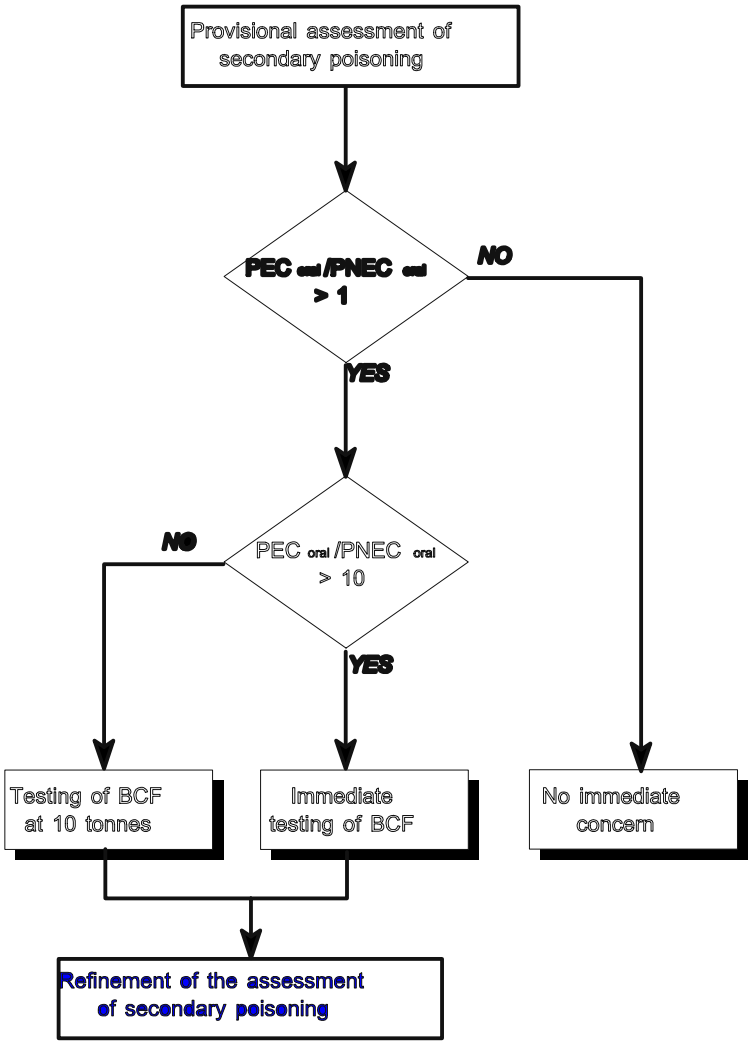

Figure 15 *Decision scheme for risk characterisation for secondary poisoning for new chemicals*

4.5 Risk characterisation when a PEC and/or PNEC cannot be calculated

Although the use of quantitative PEC/PNEC ratios is the preferred procedure for carrying out an environmental risk assessment it may be possible that either PEC or PNEC cannot be properly calculated. In that case the risk characterisation shall entail a qualitative evaluation of the likelihood that an effect will occur under the expected conditions of exposure (see Annex III, par. 4.2 of Directive 93/67/EEC).

If a qualitative exposure assessment indicates that no environmental compartment is likely to be polluted, the substance should be automatically set aside as of no immediate concern. However, if a qualitative exposure assessment indicates that environmental exposure is likely, the risk characterisation will entail consideration of the special factors mentioned in section 4.4. or section 4.3.

Depending on which and how many of those factors apply, a decision should be made on which of the options set out in Article 3.4 of Directive 93/67/EEC or Article 5 of Regulation 1488/94 is applicable.

For some substances it may not be possible to undertake a full quantitative risk assessment, using a $PEC_{water}/PNEC_{water}$ ratio because of the inability to calculate a $PNEC_{water}$. This can occur when no effects are observed in short-term tests. However, an absence of short-term toxicity does not necessarily mean that a substance has no long-term toxicity, particularly when it has a low water solubility and/or high hydrophobicity. For such substances, the concentration in water (at solubility) may not be sufficient to cause short-term effects because the time to reach a steady-state between the organism and water is longer than the test duration.
For these substances it is therefore 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 (PEC_{local} or $PEC_{regional}$, as appropriate) as well as of the probability that long-term effects may occur despite the absence of short-term effects. Thus, especially for non-polar organic compounds substances with a potential to bioaccumulate (log Kow > 3) the need for long-term testing is more compelling. For ionised substances or surfactants the determination of a trigger value on the basis of other physico-chemical properties, e.g. Kd should be sufficient to ask for long-term tests.

Taking this all into account, long-term toxicity tests are asked for immediately for substances with log Kow > 3 (or BCF > 100) and a PEC_{local} or $PEC_{regional}$ > 1/100th of the water solubility.

The water solubility should, where possible, be based on the solubility in the aquatic toxicity test water rather than distilled water (presuming that this solubility is measured after filtration (0.45 μm) of the test solution or after centrifugation). When the logKow is not a good indicator of bioconcentration, or where there are other indications of a potential to bioconcentrate (see section 3.8), a case-by-case assessment of the presumable long-term effects will be necessary.

5. Testing strategies

5.1 Refinement of PEC

In order to refine the PEC, apart from comprehensive information on production and application, additional tests may lead to a better quantification of the elimination processes of a substance in the individual environmental compartments or in the sewage treatment plant. The exact degree of elimination may be determined by measurements in the influent and effluent of sewage treatment plants or by conducting appropriate tests on the degradation behaviour. A degradation testing strategy for the environmental compartments is given below. Similarly, the experimental determination of the BCF can be requested in order to refine the PEC_{oral} for secondary poisoning (see section 3.8).

Another possible option for the refinement of the PEC is the performance of simple monitoring (for example at point of release or in predicted worst-case environments). Long-term monitoring programmes should only be initiated:

- in the case of borderline risk assessments, where immediate risk reduction action cannot be justified;
- as a means of checking the effectiveness of risk reduction action;
  taking into account monitoring programmes established under other EU legislation.

5.1.1 Aquatic compartment

In the following, a biodegradation testing strategy for the aquatic environment is presented. However, it should also be considered at each stage whether further abiotic testing, e.g. direct or indirect aquatic photolysis, full adsorption/desorption test, could refine the PEC (local or regional).

Two cases can be distinguished:

<u>PEC/PNEC > 1 and the substance is readily biodegradable</u>
Further biotic testing is unlikely to affect the PEC, unless the producer/importer believes it is worth conducting a simulation test, which may generate a removal percentage greater than that assumed for readily biodegradable substances.

<u>PEC/PNEC > 1 and the substance is not readily biodegradable</u>
If the substance is inhibitory at a level below that used in the ready test, the ready test should be repeated at a non-inhibitory concentration. This will only help refine PEC_{local} if the concentration predicted in the treatment plant is below the inhibition threshold.

However, it is likely that the result could be used in the consideration of $PEC_{regional}$. If there are indications from the test for ready biodegradation that the substance may be inherently biodegradable, then consideration should be given to the conduct of a suitable test to demonstrate this, e.g. OECD Guidelines 302B (Zahn-Wellens) or 302C (MITI II). Before requesting such a test, however, due attention should be paid as to whether the results of the test will lead to a revision of the PEC, and if so whether such a revision would likely to affect the overall conclusion of the risk characterisation. Revision of a PEC_{local}, for example, can only be achieved if the results of the inherent test show degradation according to the criteria set out in section 2.3.7.

Prior to simulation testing it may be useful to conduct a Zahn-Wellens test or a similar inherent test in order to obtain a first indication of the likely biodegradability behaviour of the compound. It is emphasised that an inherent test cannot replace simulation testing but mainly serves the purpose of providing guidance to the investigator with regard to the planning of further studies. Therefore inherent tests are optional and are generally not recommended if the testing causes technical difficulties due to high concentrations applied (toxicity, limited solubility etc.).

Therefore, an inherent test will be difficult to justify and consideration will need to be given to the conduct of a simulation test giving relevant information on the degradation kinetics. No internationally standardised methods exist yet, so draft standard methods or protocols have to be used. The results from such testing can be used directly in the calculation of PEC for the system being simulated. Care will need to be taken, however, that the conditions of the test substance concentration, reflect those likely to be found in the relevant compartment (STP, surface water, sediment and/or soil).

5.1.2 Soil compartment

If the PEC/PNEC ratio for the soil compartment is greater than one, further degradation testing will refine the assessment in several ways:

- The estimation of the amount of substance entering the soil compartment via land-spreading of sludge can be refined by more sophisticated degradation or adsorption/desorption testing in the aquatic environment;
- It can also be refined by investigating the potential for anaerobic degradation in the sludge, which is otherwise assumed to have no effect on the concentration of the substance. For testing of anaerobic biodegradation a draft guideline is now available (ISO Draft 11734). This screening test method is designed to investigate the potential for anaerobic degradation in STP digesters. In future these test results might be used to estimate anaerobic biodegradation in sediment. However, tests for anaerobic degradation and inhibition are sufficiently well developed to be considered in the risk characterisation;

- A refined estimation of the fate of the substance once it has reached the soil compartment may also be possible using [ready, inherent or simulation] tests performed in soil, provided that interpretable test methods are available, and the results have the possibility of altering the conclusion of the risk characterisation;
- Abiotic testing should also be considered. Tests include (direct) photolysis, and more refined adsorption/desorption in soil.

5.1.3 Air compartment

For the air compartment experimental testing of direct photodegradation and chemical reactions originating in atmospheric photochemistry is complicated and should only be required if there is a serious indication of possible adverse effects related to the PEC in the atmosphere. Instead it is preferable to use QSARs where they are available.

5.2 Refinement of PNEC: strategy for further testing

5.2.1 Introduction

A detailed strategy for further testing in order to refine the PNEC has been developed for the aquatic compartment. A guidance for the decision on further testing, less specific than the one for the aquatic environment, is also provided for the terrestrial compartment and for secondary poisoning. Basically, the additional tests to be conducted are long-term tests, as a PNEC based on long-term ecotoxicity data is more reliable than a PNEC based on short-term data. The additional tests lead to lower assessment factors due to the lower uncertainty. These strategies are described in detail within the discussion on the effects assessment (section 3) under the relevant compartment.

The refinement of the $PNEC_{water}$ for the aquatic compartment can be carried out by performing long-term tests with the most sensitive species or, if one or two NOEC(s) is/are already available, with a long-term test on species of trophic levels for which no NOEC was determined so far. The decision taking process can be supported by using (Q)SARs. The testing strategy is described in section 5.2.2.

The risk assessment concept for the terrestrial compartment includes also a strategy when to carry out short-term toxicity tests on terrestrial organisms as these are not included in the base-set. Short-term tests shall be conducted, if a potential risk to soil has been identified on the basis of a risk characterisation using the equilibrium partitioning method. Expert judgement is required to decide on the most appropriate long-term test(s) in order to refine the $PNEC_{soil}$, if necessary (see section 5.2.3).

While any possible refinement of the $PEC_{oral}/PNEC_{oral}$ ratio for secondary poisoning targets more on the refinement of the PEC_{oral} rather than of the $PNEC_{oral}$, it may in some cases be more appropriate to refine the latter and conduct long-term or chronic toxicity tests. The decision on which test to conduct has to be taken on a case-by-case basis.

As no internationally accepted standardised test guidelines and/or no adequate effects assessment methods are available at present no testing strategy is proposed for the sediment and air compartment. If it is concluded that one of these compartments is at risk a decision will have to be taken on a case-by-case basis.

5.2.2 Aquatic compartment

5.2.2.1 Introduction

If the ratio $PEC_{water}/PNEC_{water}$ is greater than one, either exposure data have to be refined or further testing is required. One or more additional tests may have to be performed according to the methods laid down in Annex V to Directive 67/548/EEC or as OECD test guidelines (or equivalent guidelines) for a refined risk assessment. Only those tests which may lead to a revision of the $PNEC_{water}$ have to be performed. In some circumstances, a mesocosm or (semi)field test which uses sensitive and ecosystem-specific endpoints different from those in single-species tests might be considered.

In revising the effects assessment by conducting additional aquatic toxicity testing, care must be taken to ensure that species sensitivity is fully taken into account. Although the choice of tests is necessarily limited, it must reflect the anticipated exposure conditions and the chemistry of the substance.

In determining whether additional testing is required, the following guidelines should be taken into account:

- Further testing should be directed at revising the $PNEC_{water}$ and thus lead to a recalculated $PEC_{water}/PNEC_{water}$ ratio.
  This is a key requirement in deciding whether a test is necessary. Additional testing should lead to a revision of the estimated $PNEC_{water}$ which, when based on long-term ecotoxicity data, is more reliable than when based on short-term data;
- The species with the lowest $L(E)C_{50}$ in short-term studies should normally be examined first for the purposes of long-term testing. Differences in $L(E)C_{50}$s can be determined by comparing their values: one value is considered to be significantly lower than another if it is more than ten times lower. These definitions can only provide a guide as to the relative sensitivities of taxonomic groups, however, and expert judgement must be used to determine whether they are sufficient in any given case;

- Further testing would not normally be required on a species for which no short-term toxicity has been demonstrated ($L(E)C_{50}$ > 100 mg/l). This may not apply to poorly water soluble substances (water solubility < 1 mg/l) for which no short-term toxicity may have been demonstrated (see section 4.5). In other cases, expert judgement should be used to determine whether further testing of a species is necessary.

For substances which bioaccumulate or have a potential to bioaccumulate, it should be recognised that long-term or delayed effects are possible which might not have been apparent or predicted from the short-term studies or long-term tests appropriate for non-bioaccumulating substances. This is considered to be of particular importance when considering long-term fish and Daphnia toxicity since several sensitive stages of their development can be affected because of the high lipid fraction in the early stages of their life cycles. Care needs to be taken, therefore, to ensure that the appropriate long-term test is selected so that steady state concentrations are achieved in the organisms tested for a sufficient period of time and the potential effects of bioaccumulation can be investigated. Normally, for these substances, a Fish Early Life Stage (FELS) test would be selected when examining for fish toxicity, although the 28-day growth test (log Kow < 5) or egg and sac-fry stage test (log Kow < 4) may also be considered.

The results from these long-term toxicity tests cannot exclude the possibility of delayed effects, however, and when such effects are suspected, it may be appropriate to consider full life cycle tests for fish according to the US EPA guideline 670/4-73-001 or 600/9-78-010 and/or Daphnia (A standard guideline for a full life cycle test for Daphnia is not available as yet). Such testing would not be regarded as normal and should be necessary only in exceptional circumstances.

Even with this complex information retarded effects in the ecosystems cannot be ruled out as not all ecotoxicological endpoints (such as multi-generation effects or behavioural disturbances) are recorded and the natural biomagnification process can hardly be reproduced in laboratory scale experiments.

5.2.2.2 Available long-term tests

The long-term tests available when seeking to refine the effects assessment are limited, but it is nevertheless important that the correct test is chosen to maximise the usable information and avoid unnecessary repeat testing.

Long-term fish testing

Fish early-life stage (FELS) test (OECD 210)
This test is considered as the most sensitive of the fish tests, covering several life stages of the fish from the newly fertilised egg, through hatch to early stages of growth. This is felt to cover most, but not all, of the sensitive points in the life-cycle, and is the only suitable test currently available for examining the potential toxic effects of bioaccumulation, apart from the full life cycle test. It is, however, a long test, typically 60 days post-hatch for rainbow trout (*Oncorhynchus mykiss*), or approximately 30 days post-hatch for warm water fish, and is consequently the most expensive of those available. It should be requested where long-term fish toxicity data are required and the substance has the potential to bioaccumulate.

Egg and sac-fry stage test (draft guideline)[2]
This test measures the sensitive early life stages from the newly fertilised egg to the end of the sac-fry stage. It is considerably shorter, and hence cheaper, than the FELS test but is also considered to be less sensitive. The method is currently the subject of discussion at OECD, and is available as a draft method. It offers an alternative to the FELS test for substances with log Kow less than 4. The conditions under which the egg and sac-fry stage test can be used in place of the FELS test may be clarified following the further discussion at the OECD.

28-day growth test (draft guideline)[2]
This test measures the growth of juvenile fish over a fixed period, and is considered a sensitive indicator of fish toxicity. Although it is considered to be of insufficient duration to examine all the sensitive points in the fish life-cycle, it provides a shorter and cheaper option to the FELS test for substances of log Kow < 5. It is currently the subject of discussion at OECD and is available as a draft method.

Fish, prolonged toxicity test, 14-day study (OECD 204)
This test cannot be considered as a suitable long-term toxicity study since it does not examine a sensitive stage in the fish life-cycle. It is, in effect, a prolonged acute study with fish mortality as the major end-point examined. However, sub-lethal effects are monitored and the NOEC should be based on the absence of these effects. It should not be requested where a long-term fish study is required. It should only be requested where further information on possible short-term effects is considered necessary.

[2] These test may be used in the testing strategy within the limits specified. However, they are only draft guidelines and precise circumstances in which they can be considered suitable have yet to be formalised.

Long-term Daphnia testing

14-day Daphnia reproduction test (OECD 202, part II)
This test measures the juvenile production as well as parental immobility and mortality. It is frequently (and preferably) conducted over 21 days. Although it does not cover the full life cycle of Daphnia it covers the sensitive reproduction stage. It is therefore considered a sensitive long-term study. It has, however, generated a number of problems, including reproducibility, and is being revised in a new guideline.

21-day Daphnia reproduction test (revised OECD 202, part II, draft)
This test is a development of the above procedure with a number of important modifications to improve the reliability and reproducibility. It is likely to be adopted as a replacement guideline by OECD after the completion of a ring test.

Algal testing:

Algae toxicity test (EEC C3)
The algal growth inhibition test measures the inhibition of algal growth under standard conditions of light, temperature and nutrient concentrations. The test produces an EC_{50}, which can be considered as equivalent to a short-term $L(E)C_{50}$. The lowest of E_rC_{50} and E_bC_{50} (i.e. the EC_{50} measured according to the growth rate and biomass respectively, Nyholm, 1985, 1989) should be used. It is not only a multigeneration test but also measures the sublethal effect, reduction in population growth, and therefore can be considered as a true chronic test. The NOEC may therefore be used in the testing strategy.

5.2.2.3 Decision table for further testing

The decisions to be made on further testing are detailed in Table 18 and take the basic criteria above into account, although common sense must be applied to such generalised rules when considering individual situations. The decisions taken on further testing will be different depending on species sensitivity. In all cases, the algal study from the base set is first considered as a short-term study and the EC_{50} used for calculation of the $PNEC_{water}$. However, the algal study is technically a multi-generation test and thus, if there are other long-term NOEC data, the algal NOEC can be considered as a long-term NOEC in the revised assessment. Generally, this algal NOEC would not be used unsupported by other long-term data.

Chapter 4 (Use of (Q)SARs) gives full details on the use of the QSAR estimates for substances with a non-specific mode of action and on long-term fish and Daphnia toxicity within the testing strategy.

Table 18 *Decision table for aquatic toxicity testing when results from a full base-set (FBS[(a)]) using an assessment factor on the lowest $L(E)C_{50}$, show that PEC/PNEC>1*

Variation in base-set data		**Further testing**	**Data available for assessment**	**Assessment factor[(b)]**
No significant difference between the $L(E)C_{50}$ values of fish, Daphnia or algae	A1	Long-term fish test + long-term Daphnia test + determination of NOEC algae	FBS + algae + Daphnia + fish	10
Fish LC_{50} more than 10 times lower than $L(E)C_{50}$ of Daphnia and algae	A2	Long-term fish test + determination of NOEC algae If S/L[(c)] ratio for fish > 20: long-term Daphnia test[(d)]	FBS + algae + fish FBS + algae + fish + Daphnia	50 10
Daphnia $L(E)C_{50}$ more than 10 times lower than $L(E)C_{50}$ of fish and algae	A3	Long-term Daphnia test + determination of NOEC algae If S/L[(c)] ratio for Daphnia > 20: long-term fish test[(d)]	FBS + algae + Daphnia FBS + algae + fish + Daphnia	50 10
Algae $L(E)C_{50}$ more than 10 times lower than $L(E)C_{50}$ of fish and Daphnia	A4	Test on other algae species + long-term fish/Daphnia test[(e)]	FBS + two algae[(e)] + fish/Daphnia	10[(e)]
Fish LC_{50} more than 10 times higher than $L(E)C_{50}$ of Daphnia and algae	A5	Long-term Daphnia test + determination of NOEC algae If S/L[(c)] ratio for Daphnia >20; long-term fish test[(d)]	FBS + algae + Daphnia FBS + algae + fish + Daphnia	50 10
Daphnia $L(E)C_{50}$ more than 10 times higher than $L(E)C_{50}$ of fish and algae	A6	Long-term fish test + determination of NOEC algae If S/L[(c)] ratio for fish >20: long-term Daphnia test[(d)]	FBS + algae + fish FBS + algae + fish + Daphnia	50 10
Algae $L(E)C_{50}$ more than 10 times higher than $L(E)C_{50}$ of fish and Daphnia	A7	Long-term Daphnia test + long-term fish test + determination of NOEC algae	FBS + algae + fish + Daphnia	10

NOTES:

(a) FBS = full base set which includes $L(E)C_{50}$ values for fish, Daphnia and algae.

(b) AF = the assessment factor must be applied to the lowest NOEC available at this stage, including the NOEC from the algae test.

(c) S/L refers to the short-term to long-term ratio, i.e. the ratio between the $L(E)C_{50}$ from a short-term test and the NOEC from a long-term test.

(d) Generally testing of a third species will be unnecessary since the toxicity results from the first species should be protective. However, this cannot be a fixed rule given the toxicity variations within taxonomic groups as well as between them. Thus if a short-term $L(E)C_{50}$: long-term NOEC ratio > 20 is found for the species tested, or from the algal study, then further testing of a third species might be necessary. The use of long-term fish or Daphnia QSARs could help in deciding which species need to be tested (see Chapter 4 "Use of QSARs"). It is considered that such a ratio may be indicative of an abnormal level of toxicity or a specific mode of action, and thus the acquisition of additional evidence is justified in order to improve the confidence in the calculated $PNEC_{water}$. Other factors such as the shape of the toxicity time curve and the presence of sub-lethal effects in the short-term toxicity study for the second species may also be considered. An assessment factor of 10 may be applied to the lowest of the three NOECs. Before a toxicity study on a third species is requested, due consideration should be given to whether the resultant NOEC will lead to a further revision of the $PNEC_{water}$.

(e) This table is based on the presumption that an algal NOEC is available at the base-set. If this is not the case an assessment factor of 50 should be used .

5.2.3 Soil compartment

At the moment there is a lack of standardised ecotoxicity tests for terrestrial organisms. The OECD tests on plants and earthworms are the only ones which are directly related to the soil compartment. These tests are of relatively short duration and should be regarded as short-term tests.
Several research programmes have been started in the last years, aimed at the development of soil tests: the Netherlands Integrated Soil Research Programme (NISRP; Eijsackers, 1989) and the Swedish Mark Test System (MATS; Rundgren et al., 1989). Recently, in Denmark a research programme has been started in which attention is paid to terrestrial toxicity research.

Finally, within the framework of the EU Environment Programme the international research project Sublethal Effects of Chemicals on Fauna Soil Ecosystem (SECOFASE) receives funding for the development, improvement and standardisation of ecotoxicity tests with a number of terrestrial organisms (Løkke and Van Gestel, 1993). However, it is unclear at the moment how many and which ecotoxicity tests should be implemented in testing strategies for a realistic effect assessment for the soil compartment. This means that a set of tests according to the base-set for the water compartment (algae, Daphnia and fish) does not exist for the soil compartment. A test set for soil organisms could be devised to contain data on:

- primary producers (plants);
- consumers (herbivores, fungivores and saprovorous organisms);
- decomposers (litter consumers and micro-organisms).

Within the OECD Test Guidelines Programme a suitable test set for soil organisms is being developed. Within this framework Léon and Van Gestel (1994) made an inventory of existing and international test guidelines and newly developed tests. Also they made an inventory of criteria for the selection of toxicity tests, and developed a more or less standardised method for selecting tests based on a scoring system for these criteria.

In the "OECD Terrestrial Effects Working Group Meeting" in June 1995 types of terrestrial testing required for various chemicals were discussed. For "general" chemicals the following tests were recommended at an "initial stage" (OECD, 1995):

- plant test involving exposure via soil;
- test with an annelid (earthworm acute or possibly reproduction test);

and/or

- test with a soil-dwelling arthropod.

Several tests with soil organisms are summarised in Appendix VI.

With respect to the testing strategy two cases can be distinguished if it is decided to revise the $PNEC_{soil}$:

(1) If the equilibrium partitioning method is applied due to the absence of toxicity data for soil organisms and $PEC_{soil}/PNEC_{soil}$ is >1, short term tests on primary producers, consumers and decomposers should be performed. Test guidelines are available for primary producers (OECD 208) and for consumers (OECD 207). Tests for decomposers have been developed for plant protecting agents and are available in several EU Member States as tests standardised on a national level (e.g. NEN (1988) in the Netherlands, BBA (1990b) in Germany). Currently, more methods are being developed (see Appendix VI).

(2) If the $PNEC_{soil}$ is based on toxicity data for soil organisms using assessment factors and $PEC_{soil}/PNEC_{soil} > 1$, further testing may be necessary.

Depending on the effect a substance has on vascular plants, earthworms or micro-organisms, the information about the ecotoxicological effect on the most sensitive group of organisms (primary producers, consumers or decomposers) has to be improved by conducting appropriate tests for the respective endpoints. The choice of test species will be made on a case-by-case basis taking into account the availability of a suitable test method, the indicative nature of the assessment factors and the uncertainty in the proposed approach.

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Appendix I: Emission factors for different use categories

This appendix consist of:
- release tables (A and B),
- a list of synonyms for functions of substances to obtain the best entry to the A- and B-tables (Appendix I-a and Appendix I-b),
- scheme for use of all relevant emission data for a substance (Appendix I-c).

1. Introduction to the release tables

For all industrial categories distinguished in Chapter 5 estimates have been generated for:

1. The emission factors for all (relevant) stages of the life cycle, i.e. (1) production, (2) formulation, (3) processing, (4) private use and (5) recovery; these estimates have been collected in the "A-tables".
2. The fraction of the main source and the number of emission days (point sources); these estimates have been collected in the "B-tables".

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. 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 in Chapter 7 (use category documents)) to provide a solid basis for the estimates.

2. Types of substances and levels of production and use

New substances are usually produced at a rather low level. For existing substances also high production volume chemicals (HPVC) have to be considered. The OECD list of HPVCs contained about 1600 chemicals which are either produced in excess of 10,000 tonnes in any one member country or in two or more countries in excess of 1,000 tonnes in 1990. For the B-tables, default values for every industrial category have been introduced, above which a chemical is considered to be an HPVC (unless the chemical is considered as an HPVC by the notifier). In Appendix I-c this is presented in 1: Characterisation. If the (production) volume of a substance is rather high (HPVC), it may be unrealistic to use the standard size for the STP. A correction may be made in a more refined stage of the assessment.

In the text the term "volume" will be used instead of "production volume", as the volume applied in the EU is considered now. This means that the volume equals the production volume + the volume imported in the EU - the volume exported from the EU (the substance as such, not the quantities imported in products). This is presented in Appendix I-c in 2: Tonnage.

A chemical can have applications in more than one industrial category (IC) and/or use category (UC). As an assessment has to be made for all relevant applications of the chemical, the input of fractions for different industrial and use category combinations must be realised according to 3: Use and stages of the life cycle in Appendix I-c.

3. Aspects of production

If specific data on emissions at production are known, these can be used instead of the tables (see Appendix I-c under 4: Production characteristics at "Specific emission information"). Also for the fraction of the main source specific data may be entered, either as the capacity (tonnes/day) or as the period (days/year) in which the chemical is produced (see Appendix I-c under 4: Production characteristics at "Production capacity").

4. Aspects of formulation

Also for this stage of the life cycle specific data may be entered on the fraction of the main source and the emissions/emission factors, see Appendix I-c under 5: Formulation characteristics. For the emissions, a refinement may be achieved by discriminating between cleaning with/without water and soap. This has not been done yet. In case a substance is applied in a formulation at a rather low level, unrealistic values for the fraction of the main source and the number of days will be derived from the tables using the tonnage as such. Therefore a correction should be made; a suggestion is to correct the tonnage as input for the B-table in the following way. 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. There is a possibility to calculate an average in case a range of contents has been specified. This has been worked out in Appendix I-c in 5: Formulation characteristics at "Content in formulated product".

5. Aspects of processing

Specific data on the fraction of the main source and the emissions may be used as input (see Appendix I-c in 6: Processing characteristics). This will be repeated for every specified IC-UC combination. In case a specific scenario for an IC-UC combination exists, specific data will be asked. An interesting point which is not worked out yet, is the possible emissions of chemicals which after processing will be present in articles. These articles will be used for periods ranging from days up to many years. Examples are plasticisers in PVC articles. The amount of theses articles will build up over the years, and the diffuse emissions due to migration followed by evaporation and leaching will hence increase.

6. Aspects of private use

Specific data on the fraction of the main source and the emissions may be used (see Appendix I-c in 6: Private use characteristics). This will be possible for every specified IC-UC combination for which the stage of private use is relevant.

7. Aspects of recovery

Specific data on the fraction of the main source and the emissions may be used (see Appendix I-c in 6: Recovery characteristics). This will be possible for every specified IC-UC combination for which the stage of recovery is relevant.

8. Interpretation and use of the classification in 'Main categories'

The categorisation procedure outlined in Chapter 5 allows for one entry of the Main category (MC) only, for all stages of the life cycle. The approach of MCs is however, used in many tables for more than one stage. The interpretation differs often for the stage considered and are specified below:

MC	Stage	Interpretation
1a	Production	Non-isolated intermediates (IC=3, UC=33)
1b	Production	Isolated intermediates stored on-site, or substances (other than intermediates) produced in a continuous production process
1c	Production	Isolated intermediates stored off-site, or substances (other than intermediates) produced in dedicated equipment
2	Formulation	Inclusion into or onto a matrix
	Processing	Inclusion into or onto a matrix
3	Formulation	Multi-purpose equipment
	Processing	Non-dispersive use (industrial point sources)
4	Processing	Wide dispersive use (many small point sources or diffuse releases; normally no emission reduction measures)

Remarks on the industrial category (related to the Emission Scenario Document in Chapter 7)

1. Agricultural industry

There are no emission scenario 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, e.g. UC=19 Fertilisers and UC=41 Pharmaceuticals.

2. Chemical industry: basic chemicals

There are no emission scenario documents for this IC. In case a basic chemical is formulated A- and B-tables have been provided. Recovery is not considered as a separate 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 so far; apart from UC=48 Solvents most chemicals will have to be classified as UC=43 Process regulators or UC=0 Others.

3. Chemical industry: chemicals used in synthesis

Apart from UC=33 Intermediates also in this IC most chemicals will have to be classified as UC=43 Process regulators or UC=0 Others. Formulation may be feasible for some chemicals, whilst recovery is unlikely.

4. Electrical/electronic industry

There are no emission scenario documents for this IC. There are many different applications however in this IC, e.g. at the production of printed circuits and the application of dielectric fluids in transformers and capacitors. The only distinction is between chemicals included into or onto a matrix (MC=2) and others used at point sources (MC=3) in a process.

5. Personal/domestic

Chemicals used in this IC in many cases will be present in formulations, e.g. in cleaners (soaps, detergents, washing powders, etc.) and products for the care of leather, textile and cars. Emissions will be very diffuse and only for waste water the emissions to an STP are regarded as a point source situation (assuming a more or less same usage by populations and an equal usage during the week and seasons). For products like fuels and fuel additives the emissions are calculated in IC=9 Mineral oil and fuel industry at the stage of private use. For paint products and photochemicals this is done in IC=14 Paint, lacquers and varnishes industry and IC=10 Photographic industry respectively.

6. Public domain

Most chemicals used in this IC will be present in formulations, e.g. in "cleaners" (UC=9 Cleaning and washing agents and disinfectants), non-agricultural pesticides (UC=39 Pesticides, non-agricultural) and products for the maintenance of roads, buildings, etc. For UC=9, UC=39 and all other UCs a differentiation in the number of days (B-tables) and the emission factors (A-tables) has been made.

7. Leather processing industry

No adequate emission scenario document was available, apart from a proposal by UBA, based on information by ETAD (leather dyeing). A general scenario is presented with default values in the tables for common functions of chemicals such as tanning agents (UC=51). For specific UCs (UC=6 Anti-set off and anti-adhesive agents, UC=9 Cleaning/washing agents and disinfectants, UC=10 Colorants and UC=31 Impregnation agents) different value are used.

8. Metal extraction, refining and processing industry

Though chemicals are used in many different processes in this IC only for metalworking fluids (processing stage) emission scenario document are present. The basis for the tables is the original Dutch document.

The functions of the fluids are cooling and lubrication, so the tables have specific data for UC=29 Heat transferring agents and UC=35 Lubricants and additives.

9. Mineral oil and fuel industry
There are no emission scenario documents for this IC.

10. Photographic industry
Several emission scenario documents on this IC are available. The values in the tables are based on the Dutch document.

11. Polymers industry
Although there is a detailed emission scenario document on the processing stage of polymers by the UK this has not been implemented in the tables so far. The reactions which produce the polymers (and prepolymers such as polyesters) are considered to take place in IC=10 Polymers industry at the stage of processing (i.e. the substances from the production stage are processed by companies in IC=10). For the processing stage distinction has been made between "true" polymerisation reactions (see A-tables) and other reactions (polyadditions, polycondensations, etc.). Furthermore processing of polymerous materials (thermoplastics and thermosetting resins) are considered. In the text going along with the A-tables a short explanation has been given on the interpretation of functions of chemicals and the attached UCs. Many thermoplastics are recycled nowadays, this is however not yet taken into account.

12. Pulp, paper and board industry
There are emission scenario documents from both the UK and The Netherlands on paper production (including dyeing of paper) and recycling. The UBA document proposal was not considered yet. Specific tables have been introduced to cover the printing process which has been included in this IC.

13. Textile processing industry
The original scenario derived from the Dutch document has been used for the emission tables. There are emission scenario documents by UBA and RIVM. The UBA document uses ETAD information only which takes not in account emissions to waste water due to cleaning.

14. Paints, lacquers and varnishes industry
There is a French document on paint production and a proposal from UBA on the stage of processing (paint application). These documents have not yet been considered in the emission tables. To obtain better estimates, a discrimination is made between UCs, water based and solvent based types, and application by industries and households.

16. Engineering industry: civil and mechanical
For this IC no emission scenario documents exist. Most tables match the ones applied for chemicals classified in IC=0 Others.

0. Others
General tables have been used.

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]

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		

So the release per stage of the life cycle (in tonnes per year) can be calculated by:

1. production	$RELEASE_{1,j}$:	air	$F_{1,a}$ • PRODVOL
		water	$F_{1,w}$ • PRODVOL
		soil	$F_{1,s}$ • PRODVOL
		total	$\Sigma F_{1,j}$ • PRODVOL
	amount used:		TONNAGE
2. formulat.	$RELEASE_{2,j}$:	air	$F_{2,a}$ • TONNAGE
		water	$F_{2,w}$ • TONNAGE
		soil	$F_{2,s}$ • TONNAGE
		total	$\Sigma F_{2,j}$ • TONNAGE
	rest:		$(1-\Sigma F_{2,j})$ • TONNAGE
3. processing	$RELEASE_{3,j}$:	air	$F_{3,a} \cdot (1-\Sigma F_{2,j})$ • TONNAGE
		water	$F_{3,w} \cdot (1-\Sigma F_{2,j})$ • TONNAGE
		soil	$F_{3,s} \cdot (1-\Sigma F_{2,j})$ • TONNAGE
		total	$\Sigma F_{3,j} \cdot (1-\Sigma F_{2,j})$ • TONNAGE
4. private use	$RELEASE_{4,j}$:	air	$F_{4,a}$ • $(1-\Sigma F_{2,j})$ • TONNAGE
		water	$F_{4,w}$ • $(1-\Sigma F_{2,j})$ • TONNAGE
		soil	$F_{4,s}$ • $(1-\Sigma F_{2,j})$ • TONNAGE
		total	$\Sigma F_{4,j}$ • $(1-\Sigma F_{2,j})$ • TONNAGE
		rest:	$(1-\Sigma F_{3,j} - \Sigma F_{4,j})$ • $(1-\Sigma F_{2,j})$ • TONNAGE

5. recovery	$RELEASE_{5,j}$:	air	$F_{5,a} \bullet (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \bullet (1-\Sigma F_{2,j}) \bullet TONNAGE$
		water	$F_{5,w} \bullet (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \bullet (1-\Sigma F_{2,j}) \bullet TONNAGE$
		soil	$F_{5,s} \bullet (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \bullet (1-\Sigma F_{2,j}) \bullet TONNAGE$
		total	$\Sigma F_{5,j} \bullet (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \bullet (1-\Sigma F_{2,j}) \bullet TONNAGE$

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.(1) (Ch.2)
$RELEASE_{i,j}$	release during life cycle stage *i* to compartment *j*	[tonnes.yr^{-1}]	

A-tables

Estimates for the emission factors (fractions released)

IC = 1: AGRICULTURAL INDUSTRY

PRODUCTION Table A1.1

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1b	MC=1c	MC=3 (1)
Air		<1		0	0	0.00001
		1-10		0	0.00001	0.0001
		10-100		0.00001	0.0001	0.001
		100-1,000		0.0001	0.001	0.01
		1,000-10,000		0.001	0.005	0.05
		≥10,000		0.005	0.01	0.05
	T (tonnes/year)					
Waste water	<1,000		0.02			
	≥1,000		0.003			
Soil			0.0001			

(1) Default

FORMULATION Table A2.1

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1b	MC=1c	MC=3 (1)
Air		<10		0.0005	0.001	0.0025
		10-100		0.001	0.0025	0.005
		100-1,000		0.0025	0.005	0.01
		≥1,000		0.005	0.01	0.025
		T (tonnes/year)				
Waste water		<1,000	0.02			
		≥1,000	0.003			
Soil			0.0001			

(1) Default

PROCESSING Table A3.1*

UC's	Description	Emission factors to: Air	Surface w.	Soil
Default		0.1	0.1	0.8
3	areosol propellants	1	0	0
9, 10, 36	cleaning/washing agents and additives + colorants + odour agents	0	0.1	0.4
19	fertilisers	0	0.05	0.95
26	food/feedstuff additives	0	0	0.05
38, 50	pesticides + surfactants	0.05	0.1	0.85
41	pharmaceuticals (external application)	0	0	0.1
41	pharmaceuticals (internal application)	0	0	0
48	solvents	1	0	0

PRIVATE USE Not applicable
RECOVERY Not applicable

* Fertilisers and pesticides + surfactants go to agricultural soil on the regional and continental scale, the others go to industrial soil

IC=2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.2

Conditions		Emission factors		
Sol. (mg/l)	Vap. (Pa)	Air	Waste water	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

RECOVERY Not applicable
(Emissions at recovery of chemicals such as catalysts are included in the emissions at processing)

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
	T (tonnes/year)					
Waste water	<1,000		0.02			
	≥1,000		0.003			

PRODUCTION Table A1.2 for UC = 33 (intermediates) **Continued**

Compartment	Conditions	Emission factors			
		All MC's	MC=1a	MC=1b	MC=1c
Soil			0	0.00001	0.0001

FORMULATION Table A2.1

PROCESSING 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
	T (tonnes/year)					
Waste water	<1,000		0.02			
	≥1,000		0.007	0.0005		
Soil			0.0001			

(1) Default

Remark: The releases at processing 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
RECOVERY Not applicable

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.4

Compartment	Conditions		Emission factors	
	Sol. (mg/l)	Vap. (Pa)	MC = 2	MC = 3 (1)
Air		<100	0.0005	0.0005
		≥100	0.0005	0.001
Waste water			0.0001	0.005

PROCESSING Table A3.4 **Continued**

Compartment	Conditions		Emission factors	
	Sol. (mg/l)	Vap. (Pa)	MC = 2	MC = 3 (1)
Soil			0.0001	0.01

PRIVATE USE Not applicable

RECOVERY Not applicable

IC = 5: PERSONAL /DOMESTIC

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING 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, 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
	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

PRIVATE USE Table A4.1 **Continued**

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Air	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
		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
		≥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
Waste water	2	<25		0
		≥25		0.005
	3, 5, 19, 35			0
	7			0.01
	8 (household products)			0.95
	(cosmetics)			0.8
	9, 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, etc.)		<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
	38 (herbicides)			0
	(pesticides, garden)			0
	(pesticides, pets)			0.1

PRIVATE USE Table A4.1 **Continued**

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Waste water	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, 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

RECOVERY Not applicable

IC = 6: PUBLIC DOMAIN

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.5

Conditions Use categories		Emission factors Air	Waste water	Soil
9	(cleaning/washing agents)	0.0025	0.9	0.05
39	(non-agric. pesticides)	0.1	0.05	0.8
All	other	0.05	0.45	0.45

PRIVATE USE Not applicable

RECOVERY 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)	Vap. (Pa)	Emission factors
Air			0.0008
Waste water	<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

PROCESSING Table A3.6

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC = 2	MC = 3 (1)
Air	<100	<100	0.001		
	<100	≥100	0.01		
	≥100		0		
Waste water	<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

RECOVERY 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 Sol. (mg/l)	Vap. (Pa)	Emission factors
Air		<1	0.00005
		1-10	0.00001
		10-100	0.0005
		100-1,000	0.0025
		≥1,000	0.025
Waste water			0.002
Soil			0.00001

(1) Default

PROCESSING Table A3.7

Compartment	Conditions UC≠29&35	Sol. (mg/l)	Emission factors MC = 2	MC = 3 (1)
Air			0	0.25
Waste water		<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
Waste water	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

RECOVERY Not applicable

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.8

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors
Air		<1	0.0001
		1-10	0.0005
		10-100	0.001
		100-1,000	0.005
		≥1,000	0.01
Waste water			0.0005
Soil			0.001

PRIVATE USE Table A4.2

Compartment	Conditions Vap. (Pa)	Emission factors
Air	<10	0.005
	10-100	0.015
	100-1,000	0.15
	1,000-10,000	0.4
	≥10,000	0.6
Waste water		0.0005
Surface water		0.0001
Soil		0.0001

RECOVERY Not applicable

IC = 10: PHOTOGRAPHIC INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1 default for formulations to be used in photographic baths
Table A2.1 must be used for aqueous solutions, Table A2.3 for solid materials

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors
Air		<1	0.0001
		1-10	0.001
		10-100	0.3
		100-1,000	0.7
		≥1,000	1

FORMULATION Table A2.3 for UC=42, and other UC's in the manufacture of solid materials **Continued**

Compartment	Conditions	Emission factors
Waste water	Control of crystal growth	1
	Other functions	0.002
Soil		0.00025

(1) Default

PROCESSING Table A3.9

Compartment	Conditions	Vap. (Pa)	Emission factors 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
Waste water	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 UC=42 (photochemicals), for aqueous solutions only!	Emission factors
Air		0
Waste water		0.4
Soil		0

RECOVERY Table A5.1

Compartment	Conditions UC=42 (photochemicals), for aqueous solutions only!	Vap. (Pa)	Emission factors
Air		<1	0.000005
		1-10	0.000025
		10-100	0.00075
		100-1,000	0.0025
		≥1,000	0.01
Waste water			0.2
Soil			0

IC = 11: POLYMERS INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING 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

PROCESSING Table A3.10 for polymerisation processes **Continued**

Compartment	Conditions	Emission factors					
		Type I		Type II		Type III	
	Sol. (mg/l)	"Wet"	"Dry"	"Wet"	"Dry"	"Wet"	"Dry"
Waste water	<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

PROCESSING Table A3.11 for polymer processing

Processing of polymers ("shaping" by all kind of techniques) occurs in many Industrial categories

Two categories of polymer processing are distinguished:
A Processing of thermoplastics
B Processing of thermosetting resins (prepolymers)

For the emission factors the following types of chemicals used are considered:

I	(A, B)	Additives	UC 7 (Anti-static agents), 22 (Flame retardants), 49 (Stabilisers) & 55 Others (e.g. antioxidants)
		Pigments	UC 10 (Colorants)
		Fillers	UC 20
II	(A)	Plasticisers	UC 47 (softeners)
III	(A, B)	Solvents	UC 48
IV	(A, B)	Processing aids	UC 6 (Anti-set off and anti-adhesive agents) & 35 (lubricants and additives)
V	(B)	Curing agents	UC 43 (Process regulators, e.g. initiators)
		Cross-linking agents	UC 43 (Process regulators: monomers)

Compartment	Conditions Vap. (Pa)	Boiling point (°C)	Emission factors A	B	Type of chemicals
Air	<1	<300/unknown	0.001	0	I
		≥300	0.0005	0	
	1-100	<300/unknown	0.0025	0	
		≥300	0.001	0	
	≥100	<300/unknown	0.01	0	
		≥300	0.005	0	
		<400/unknown	0.01		II
		≥400	0.005		
	<100		0.1	0.1	III
	100-1,000		0.25	0.25	
	1,000-10,000		0.5	0.5	
	≥10,000		0.75	0.75	

PROCESSING Table A3.11 for polymer processing **Continued**

Compartment	Conditions Vap. (Pa)	Boiling point (°C)	Emission factors A	B	Type of chemicals
Air	<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	
Waste water			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

RECOVERY 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)

PROCESSING — Table A3.12 for printing and allied processes

Compartment	Conditions Use categories		Emission factors MC = 2	MC = 3 (1)
Air	Default	Vap. (Pa)		
		<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)
Waste water	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

PROCESSING Table A3.12 for pulp, paper and board production

Compartment	Conditions Use category		Emission factors 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	

PROCESSING Table A3.12 for pulp, paper and board production **Continued**

Compartment	Conditions Use category		Emission factors Sol. (mg/l)	Vap. (Pa)	MC=2	MC=3 (1)
Waste water	Default	<100	<100		0.85	
			100-500		0.75	
			≥500		0.5	
		100-1,000	<100		0.875	
			100-500		0.85	
			≥500		0.75	
		1,000-10,000	<100		0.9	
			100-500		0.875	
			≥500		0.85	
		≥10,000	-		0.95	
	10:					
	- Basic dye, anion			0.023		
	- Direct dye				0.04	
	- Direct dye, kation			0.055		
	- Direct dye, anion/kation			0.028		
	- Acid dye, kation/unknown				0.079	
	- Brightener				0.064	
	20 & 31			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

RECOVERY Table A5.2

Compartment	Conditions	Emission factors
Air		0
Waste water	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

PROCESSING Table A3.14

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	UC = 10
Air	<100	<100	0.95	
		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	
	Conditions			
	Batch dyeing			0.0007
	Continuous dyeing			
	- thermosol/unknown			0.05
	- other			0.0025
	- printing			0.0025

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	UC = 10
Waste water	<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	<100	0.95	

WASTE WATER 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 * B) B = 1 / liquor ratio (liquor ratio: default = 10 kg fibres / 1 l solution)
A = constant
K = equilibrium constant

PROCESSING Table A3.14 **Continued**

Conditions Type of dye	(**UC = 10**) Type of dyeing	K	A	B	E.2
Disperse	Continuous	115	5	1	0.055
"	Printing	115	2	0.5	0.12
Direct	Batch	73	1	0.1 (1)	0.01
Reactive - wool	Batch	190	1	0.1 (1)	0.01
Reactive - cotton	Batch	23	1	0.1 (1)	0.01
Reactive - general	Batch	57	1	0.1 (1)	0.01
Vat	Continuous	190	5	1	0.055
	Printing	190	2	0.5	0.12
Sulphur	Continuous	40	5	1	0.055
	Printing	40	2	0.5	0.12
Acid - one SO3	Batch	90	1	0.1 (1)	0.01
Acid - > 1 SO3	Batch	190	1	0.1 (1)	0.01
Basic	Batch	990	1	0.1 (1)	0.01
Azoic (naphtole)	Continuous	30	5	1	0.055
	Printing	30	2	0.5	0.12
Metal complex	Batch	150	1	0.1 (1)	0.01
Pigment	Continuous	5000	5	1	0.055
	Printing	5000	2	0.5	0.12
Unknown, low solubility	Continuous	190	5	1	0.055
	Printing	190	2	0.5	0.12
Unknown, acid groups	Batch	90	1	0.1 (1)	0.01

(1) Default

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	UC=10
Soil				0.005
	<100	<100	0.005	
		100-500	0.0025	
		≥500	0.001	
	≥100	<100	0.005	
		100-500	0.002	
		≥500	0.001	

PRIVATE USE Table A4.4

Compartment	Conditions Sol. (mg/l)	Emission factors UC<>10	UC=10 (1)
Air			0
Waste water	<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

5. RECOVERY Not applicable

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.15

Compartment	Conditions Use category	Vap. (Pa)	Emission factors Water based	Solvent based
Air	3			1
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48	0.8	0.9	
		Sol. (mg/l)		
Waste water	3			0
	10, 14, 20		0.005	0.001
	50	<10	0.005	
		10-100	0.01	
		≥100	0.05	
	47, 52, 0	<10	0.005	0.001
		10-100	0.01	0.005
		≥100	0.05	0.01
	48		0.1	0.02
Soil	3			0
	10, 14, 20		0.005	0.005
	50		0.005	
	47, 52, 55		0.005	0.005
	48		0.001	0.001

PRIVATE USE Table A4.5

Compartment	Conditions Use category	Vap. (Pa)	Emission factors Water based	Solvent based
Air	3		1	
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48	0.8	0.95	

PRIVATE USE Table A4.5 **Continued**

	Conditions		Emission factors	
	Use category	Sol. (mg/l)	Water based	Solvent based
Waste water	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

RECOVERY Not applicable

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING 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

Compartment	Conditions		Emission factors		
	Sol. (mg/l)	Vap. (Pa)	MC=2	MC=3 (1)	MC =4
Waste water	<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

4. PRIVATE USE Table A3.16

RECOVERY Not applicable

IC = 0: OTHERS

PRODUCTION	Table A1.1
FORMULATION	Table A2.1
PROCESSING	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)

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)

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

PROCESSING 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

RECOVERY 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

PROCESSING 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

RECOVERY 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!

PROCESSING — Table B3.2

PRIVATE USE — Not applicable

RECOVERY — 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

PROCESSING Table B3.2

PRIVATE USE Not applicable

RECOVERY 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
PROCESSING	Not applicable
PRIVATE USE *Only for waste water!*	Table B4.1

T (tonnes/year)	f main source	No. of days:
	0.002	365

RECOVERY 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

PROCESSING Table B3.3
Only for waste water!

T (tonnes/year)	f main source	No. of days for use categories: 9	39	Else
	0.002	200	15	50

PRIVATE USE Not applicable

RECOVERY 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

PROCESSING — 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
RECOVERY — 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

PROCESSING — Table B3.5 for UC = 29 & 35

T (tonnes/year)	No. of days	f main source:	Field of application Primary steelworks	Else
<1,000	300		1	0.8
1,000-5,000	300		0.9	0.5
5,000-50,000	300		0.75	0.3
≥50,000	300		0.6	0.2

PROCESSING — 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

RECOVERY — 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

PROCESSING
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 waste water!

RECOVERY
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

PROCESSING — 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 if company size at processing is small companies

T (tonnes/year)	f main source	No. of days:
<10	0	200
10-50	0.00002	200
50-500	0.0001	200
500-5,000	0.0005	200
≥5,000	0.0025	200

RECOVERY — 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

PROCESSING — 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
RECOVERY — 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
PROCESSING	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

RECOVERY 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

PROCESSING 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

PROCESSING 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

RECOVERY 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

PROCESSING — 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 paints classified as 'do-it-yourself'

T (tonnes/year)	f main source	No. of days:
<500	1	150
≥500	1	300

PRIVATE USE — Table B4.5*
Only for paints classified as 'constructions, maintenance', etc.

T (tonnes/year)	f main source	No. of days:
<50	0	
50-500	0.00002	200
500-2,500	0.0004	300
2,500-10,000	0.002	300
10,000-50,000	0.01	300
≥50,000	0.05	300

RECOVERY — Not applicable

* The fractions listed are fraction of the remaining tonnage, applied for private use. Since the private use is by the public at large, the STP is seen as the local point source. Therefore these fractions have to be multiplied by a factor of 0.002 to get the fraction for the point source

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
PROCESSING	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
RECOVERY	Not applicable

IC = 0 (Others)

PRODUCTION	Table B1.2 for non-HPVC Table B1.6 for HPVC (default ³7,000)
FORMULATION	Table B2.8 for non-HPVC Table B2.3 for HPVC
PROCESSING	Table B3.14
PRIVATE USE	Table B4.5
RECOVERY	Table B5.3

T (tonnes/year)	f main source	No. of days
<100	0.5	150
100-1,000	0.3	150
1,000-10,000	0.2	150
≥10,000	0.2	150

Appendix I-a: List of synonyms for functions according to ChemUSES (US-EPA, 1980)

No.	USE CATEGORY	No.	Function (ChemUSES)
1	Absorbents and adsorbents	131	Absorbents
		60	Adsorbents
		213	Dehumidifiers
2	Adhesive, binding agents	302	Adhesives
		143	Binders
		145	Food additives
		92	Spreaders
		165	Stickers
		280	Tackifiers
3	Aerosol propellants	178	Aerosol propellants
4	Anti-condensation agents		
5	Anti-freezing agents	77	Antifreezes
		74	De-icers
		52	Deodorants
		313	Functional fluids
6	Anti-set-off and anti-adhesive agents	104	Abherents
		63	Antiblocking agents
		188	Anticaking agents
		300	Detackifiers
		233	Dusting agents
		144	Parting agents
		7	Soil retardants
7	Anti-static agents	328	Antistatic agents
		89	Electroconductive coating agents
		318	Humectants
8	Bleaching agents	304	Bleaching assistants
		132	Bleaching agents
9	Cleaning/washing agents and additives	293	Antiredeposition agents
		180	Boil-off assistants
		242	Cleaners
		173	Detergents
		78	Pre-spotting agents
		274	Scouring agents
		261	Shrinkage controllers
		14	Soaping-off assistants
		294	Soil release agents
10	Colouring agents	5	Bloom agents
		86	Colouring agents
		174	Coupling agents (dyes)
		267	Dyes
		20	Fluorescent agents

10	Colouring agents (continued)	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
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
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
		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

43	Process regulators (continued)	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
		315	Crabbing assistants
		228	Crosslinking agents
		226	Curing agents (concrete)
		369	Curing agents (polymer technology)
		18	Currying agents
		236	Deasphalting agents
		342	Defoamers
		365	Degumming agents
		137	Dehairing agents
		73	Dehydrating agents
		366	De-inkers
		84	Delignification agents
		30	Depolymerisation agents
		367	Depressants
		292	Desising agents
		259	Dispersants
		317	Dryers
		150	Dye carriers
		255	Dye levelling agents
		307	Dye retardants
		211	Dye retention aids
		341	Enzyme inhibitors
		157	Enzymes
		284	Finishing agents
		337	Formation aids
		331	Fuel oxidisers
		117	Fulling agents
		103	Initiators
		359	Intensifiers (printing)
		171	Kier boiling assistants
		24	Nucleating agents
		96	Peptising agents
		75	Pitch control agents
		121	Polymerisation additives
		209	Polymerisation inhibitors
		21	Prevulcanisation inhibitors
		153	Refining agents
		223	Repulping aids
		136	Retarders
		296	Retention aids
		338	Rubber compounding agents
		51	Scavengers
		326	Solubilising agents
		310	Weighting agents (petroleum technology)
44	Reducing agents	244	Reducers
45	Reprographic agents	225	Toners

46	Semiconductors	202	Semiconductors
		378	Photovoltaic agents
47	Softeners	269	Bates
		231	Devulcanising agents
		28	Elasticisers
		265	Emollients
		185	Plasticisers
		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
49	Stabilisers (continued)	129	Antihydrolysis agents
		168	Antiozonants
		230	Antioxidants
		120	Antilivering agents
		282	Antiplasticisers
		160	Antisagging agents
		68	Antisettling agents
		88	Bloom inhibitors
		123	Coupling agents (polymers)
		159	Emulsifiers
		87	Heat stabilisers
		54	Stabilisers
		36	Ultraviolet absorbers
50	Surface-active agents	41	Antifloating agents
		234	Antifogging agents
		109	Surfactants
		243	Wetting agents
51	Tanning agents	316	Tanning agents
52	Viscosity adjustors	152	Antiflooding agents
		120	Antilivering agents
		343	Antiskinning agents
		221	Gelling agents
		262	Pour point depressants
		272	Thickeners
		334	Thixotropic agents
		240	Turbulence suppressors
		135	Viscosity adjustors
		15	Viscosity index improvers
53	Vulcanising agents	288	Vulcanising agents
54	Welding and soldering agents	101	Brazing agents
		22	Fluxing agents

0 Other

204 Ablatives
105 Abrasives
196 Activators (luminescence)
354 Aerating agents
47 Air entraining agents
376 Alloying agents
90 Anticratering agents
48 Anticreasing agents
99 Antifogging agents
218 Antipilling agents
350 Antiskid agents
6 Blasting abrasives
70 Bluing agents
220 Bright dips
93 Chemical raw materials
298 Clarifiers
260 Cloud point depressants
130 Coating agents
283 Collectors
335 Coupling agents (solutions)
215 Culture nutrients
81 Deaerating agents
309 Deblooming agents
85 Dechlorinating agents
73 Dehydrating agents
107 Deionisers
232 Demulsifiers
200 Denaturants
49 Descaling agents
205 Dewatering aids
356 Discharge printing agents
38 Drainage aids
44 Drilling mud additives
322 Dry strength additives
39 Dye stripping agents
100 Electron emission agents
340 Eluting agents
372 Embalming agents
186 Encapsulating agents
57 Enhanced oil recovery agents
308 Entraining agents
319 Etching agents
336 Evaporation control agents
373 Extraction agents
207 Fiber-forming compounds
368 Filtration aids
56 Flatting agents
79 Flavours and fragrances
142 Fluid loss additives
313 Functional fluids
193 Greaseproofing agents
184 "Grinding, lapping, sanding and"
192 Hormones
246 Humidity indicators
210 Hydrotropic agents
181 Impact modifiers
380 Incandescent agents
69 Indicators

2	Ion exchange agents
91	Lachrymators
33	Latex compounding agents
53	Leaching agents
156	Leather processing agents
370	Liquid crystals
381	Luminescent agents
379	Magnetic agents
67	Mar proofing agents
289	Metal conditioners
95	Metal strippers
37	Metal treating agents
327	Milling aids
237	Obscuring agents
197	Oil repellents
62	Optical quenchers
382	Osmotic membranes
17	Papermaking agents
55	Phosphatising agents
203	Phosphorescent agents
59	Pickling agents
217	Pickling inhibitors
251	Plant growth regulators
176	Plastics additives
224	Plastics for shaping
169	Plating agents
8	Poison gas decontaminants
3	Polymer strippers
111	Pore forming agents
151	Precipitating agents
106	Protective agents
45	Radioactivity decontaminants
374	Reagents
219	Refractive index modifiers
241	Refractories
154	Resists
9	Rinse aids
71	Ripening agents
187	Rubber for shaping
201	Rubber reclaiming agents
189	Rubbing fastness agents
276	Rust inhibitors
11	Rust removers
263	Scrooping agents
42	Sealants
98	Sizes
126	Slime control agents
305	Soil conditioners
61	Strippers
40	Tar removers
345	Tarnish inhibitors
13	Tarnish removers
279	Textile specialities
257	Vat printing assistants
273	Wax strippers
35	Well treating agents
175	Wet strength additives
377	X-ray absorbents

Appendix I-b: List of synonyms for functions according to ChemUSES (US-EPA, 1980)

No.	ChemUSES Function	Use category EU (No.)
104	Abherents	6
204	Ablatives	55
105	Abrasives	0
131	Absorbents	1
321	Accelerators	43
214	Acidulants	26
254	Acoustical insulating material	32
46	Activators (chemical processes)	43
163	Activators (ore processing)	23
196	Activators (luminescence)	55
239	Activators (enzymes)	43
110	Adhesion promoters	43
302	Adhesives	2
60	Adsorbents	1
354	Aerating agents	0
178	Aerosol propellents	3
47	Air entraining agents	0
287	Algicides	39
376	Alloying agents	0
238	Analytical and product testing	34
166	Animal repellents	38
63	Antiblocking agents	6
188	Anticaking agents	6
277	Anticracking agents	49
90	Anticratering agents	0
48	Anticreasing agents	0
291	Anticrock agents	21
4	Antifelting agents	43
41	Antifloating agents	50
152	Antiflooding agents	52
234	Antifogging agents	50
99	Antifogging agents	0
1	Antifouling agents	39
329	Antifouling agents	28
77	Antifreezes	5
12	Antifume agents	49
129	Antihydrolysis agents	49
76	Antiknock agents	28
120	Antilivering agents	49, 52
230	Antioxidants	14, 49
168	Antiozonants	49
301	Antiperspirants	15
218	Antipilling agents	55
282	Antiplasticisers	49
177	Antiprecipitants	11
293	Antiredeposition agents	9
160	Antisagging agents	49
64	Antiscaling agents	14
119	Antiseize agents	35
68	Antisettling agents	49
350	Antiskid agents	0
343	Antiskinning agents	52
352	Antislip finishing agents	43
206	Antistaining agents	43
328	Antistatic agents	7
347	Antistripping agents	21
194	Antiwebbing agents	43
333	Bactericides	38
268	Barrier coating agents	21
269	Bates	47
143	Binders	2
108	Biocides	38
6	Blasting abrasives	0
132	Bleaching agents	8
304	Bleaching assistants	8
5	Bloom agents	10
88	Bloom inhibitors	49
358	Blowing agents	25
70	Bluing agents	0
180	Boil-off assistants	9
101	Brazing agents	54
220	Bright dips	0
353	Brighteners	17
281	Builders	43
222	Carbonising agents	43
164	Carriers	43
324	Case-hardening agents	13
170	Catalysts	43
19	Catalyst supports	43
31	Chain extenders	43
113	Chain terminators	43
141	Chain transfer agents	43
122	Chelating agents	34, 42, 43
133	Chemical blowing agents	25
93	Chemical raw materials	0
298	Clarifiers	0
242	Cleaners	9
260	Cloud point depressants	0
114	Coagulants	43
278	Coalescents	43
357	Coalescing agents	43
130	Coating agents	0
283	Collectors	0
86	Colouring agents	10
124	Complexing agents	11
355	Concrete additives	13
72	Coolants	29
323	Corrosion inhibitors	14
167	Cosmetic ingredients	15
123	Coupling agents (polymers)	49
174	Coupling agents (dyes)	10
335	Coupling agents (solutions)	55
315	Crabbing assistants	43
228	Crosslinking agents	43
215	Culture nutrients	0
226	Curing agents (concrete)	43
369	Curing agents (polymer technology)	43
18	Currying agents	43
366	De-inkers	43
81	Deaerating agents	0
236	Deasphalting agents	43
309	Deblooming agents	0
85	Dechlorinating agents	55
97	Decontaminats	38
342	Defoamers	43
229	Degreasers	48
365	Degumming agents	43
137	Dehairing agents	43
213	Dehumidifiers	1
73	Dehydrating agents	0, 34
74	Deicers	5
107	Deionizers	0, 34

84	Delignification agents	43
102	Delustrants	31
232	Demulsifiers	0
200	Denaturants	0
52	Deodorants	5
30	Depolymerisation agents	43
183	Deposit modifiers	28
367	Depressants	43
49	Descaling agents	0
198	Desensitisers (explosives)	42
299	Desensitisers (photography)	42
292	Desizing agents	43
300	Detackifiers	6
173	Detergents	9
179	Detonators	18
182	Developers	42
231	Devulcanising agents	47
205	Dewatering aids	0
82	Dewaxing solvents	48
356	Discharge printing agents	0
140	Disinfectants	39
259	Dispersants	43
38	Drainage aids	0
317	Dryers	43
44	Drilling mud additives	0
322	Dry strength additives	0
26	Dust control agents	16
233	Dusting agents	6
150	Dye carriers	43
255	Dye leveling agents	43
307	Dye retardants	43
211	Dye retention aids	43
39	Dye stripping agents	0
267	Dyes	10
28	Elasticisers	47
161	Electrical conductive agents	12
311	Electrical insulating material	32
89	Electroconductive coating agents	7
383	Electrode materials	12
245	Electrolytes	12
100	Electron emission agents	0
340	Eluting agents	0
372	Embalming agents	0
361	Embrittlement inhibitors	13
265	Emollients	47
159	Emulsifiers	49
186	Encapsulating agents	0
57	Enhanced oil recovery agents	0
308	Entraining agents	0
341	Enzyme inhibitors	43
157	Enzymes	43
319	Etching agents	0
336	Evaporation control agents	0
363	Explosion inhibitors	18
158	Explosives	18
373	Extraction agents	34, 48
66	Feed additives	26
34	Fertilisers	19
207	Fiber-forming compounds	0
212	Fillers (patching)	20
351	Fillers (augmentation)	20
368	Filtration aids	0
284	Finishing agents	43
25	Fire extinguishing agents	22
295	Fixatives	21
112	Fixing agents (textile technology)	21
134	Fixing agents (fragrances)	21
332	Flame retardants	22
56	Flatting agents	0
79	Flavours and fragrances	0, 36
190	Flocculating agents	23
297	Flotation agents	23
142	Fluid loss additives	0
20	Fluorescent agents	10
22	Fluxing agents	54
145	Food additives	2
337	Formation aids	43
94	Frothers	25
306	Fuel additives	28
331	Fuel oxidisers	43
247	Fuels	27
117	Fulling agents	43
32	Fume suppressants	17
270	Fumigants	38
313	Functional fluids	0, 5, 12, 29, 30, 35
362	Fungicides	38
221	Gelling agents	52
193	Greaseproofing agents	0
184	Grinding, lapping, sanding and polishing abrasives	0
199	Heat transfer agents	29
314	Heat insulating materials	32
87	Heat stabilisers	49
275	Herbicides	38
192	Hormones	0
318	Humectants	7
246	Humidity indicators	0
65	Hydraulic fluids	30
210	Hydrotropic agents	0
181	Impact modifiers	0
380	Incandescent agents	0
27	Incendiaries	18
69	Indicators	0, 34
103	Initiators	43
146	Inorganic intermediates	33
155	Insect attractants	38
348	Insect repellents	38
330	Insecticides	38
162	Insulating materials	32
286	Intensifiers (photography)	42
359	Intensifiers (printing)	43
148	Internal lubricating agents	35
2	Ion exchange agents	0
171	Kier boiling assistants	43
91	Lachrymators	0
248	Lakes	10
33	Latex compounding agents	0
172	Laundry sours	40
53	Leaching agents	0
156	Leather processing agents	0
285	Light stabilisers	42
370	Liquid crystals	0
195	Lubricant additives	35
364	Lubricating agents	35
381	Luminescent agents	0, 10
379	Magnetic agents	0
67	Mar proofing agents	55
375	Materials for shaping	13
235	Mercerising assistants	10
289	Metal conditioners	0
37	Metal treating agents	0
95	Metal strippers	0
327	Milling aids	0
360	Modifiers	23

115	Monomers	33
227	Mordents	21
252	Nematocides	38
24	Nucleating agents	43
237	Obscuring agents	0
339	Odorants	36
197	Oil repellents	0
346	Oiliness agents	35
128	Opacifiers	10
62	Optical quenchers	0
290	Organic intermediates	33
382	Osmotic membranes	0
325	Oxidation-reduction indicators	34
149	Oxidisers	37
320	Paint and varnish removers	48
17	Papermaking agents	0
144	Parting agents	6
139	Pearlising agents	10
249	Penetrants	35
96	Peptising agents	43
253	Pesticides	38
191	pH indicators	40
266	pH control agents	40
55	Phosphatising agents	0
203	Phosphorescent agents	0
344	Photosensitive agents	42
378	Photovoltaic agents	42
50	Physical blowing agents	25
217	Pickling inhibitors	0
59	Pickling agents	0
125	Pigments	10
75	Pitch control agents	43
251	Plant growth regulators	0
185	Plasticisers	47
176	Plastics additives	0
224	Plastics for shaping	0
169	Plating agents	0
8	Poison gas decontaminants	0
3	Polymer strippers	0
121	Polymerisation additives	43
209	Polymerisation inhibitors	43
111	Pore forming agents	0
262	Pour point depressants	52
78	Pre-spotting agents	9
151	Precipitating agents	0
43	Prepolymers	33
118	Preservatives	39
21	Prevulcanisation inhibitors	43
106	Protective agents	0
216	Quenchers	29
45	Radioactivity decontaminants	0
16	Reaction media	48
374	Reagents	0, 34
244	Reducers	44
153	Refining agents	43
219	Refractive index modifiers	0
241	Refractories	0
208	Refrigerants	29
250	Reinforcing agents	13
223	Repulping aids	43
154	Resists	0
136	Retarders	43
296	Retention aids	43
9	Rinse aids	0
71	Ripening agents	0
264	Rodenticides	38
338	Rubber compounding agents	43
187	Rubber for shaping	0
201	Rubber reclaiming agents	0
189	Rubbing fastness agents	0
11	Rust removers	0
276	Rust inhibitors	0
51	Scavengers	43
274	Scouring agents	9
263	Scrooping agents	0
42	Sealants	0
202	Semiconductors	46
303	Sensitisers	42
10	Sequestering agents	11
261	Shrinkage controllers	9
98	Sizes	0, 31
126	Slime control agents	0
116	Slime preventatives	39
312	Slip agents	35
14	Soaping-off assistants	9
29	Softeners	47
305	Soil conditioners	0
294	Soil release agents	9
7	Soil retardants	6
326	Solubilising agents	43
271	Solvents	48
92	Spreaders	2
54	Stabilisers	49
83	Stains	10
165	Stickers	2
61	Strippers	0
371	Surface coating additives	20
109	Surfactants	50
138	Sweeteners (petroleum technology)	28
80	Sweeteners (taste)	26
127	Swelling agents	20
280	Tackifiers	2
316	Tanning agents	51
40	Tar removers	0
13	Tarnish removers	0
345	Tarnish inhibitors	0
279	Textile specialities	0
272	Thickeners	52
334	Thixotropic agents	52
225	Toners	45
256	Transmission fluids	30
240	Turbulence suppressors	52
36	Ultraviolet absorbers	49
257	Vat printing assistants	0
135	Viscosity adjustors	52
15	Viscosity index improvers	52
288	Vulcanising agents	53
147	Water softeners	47
258	Water repellents	31
349	Water-reducing agents	13
23	Waterproofing agents	31
273	Wax strippers	0
310	Weighting agents (petroleum technology)	43
58	Weighting agents (textile technology)	20
35	Well treating agents	0
175	Wet strength additives	0
243	Wetting agents	50
377	X-ray absorbents	0

Appendix I-c: Input scheme for emission data on substances

1. Characterisation

	Yes	No
High Production Volume Chemical	☐	☐
Other existing chemical	☐	☐
New chemical	☐	☐
Not specified		☐

2. Tonnage

A Produced (tpa): ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐

B Imported (tpa): ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐

C Exported (tpa): ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐

3. Use and stages of the life cycle

	Yes	No
Production	☐	☐

		Processing			Production		Formulation		Private use		Recovery			
No.	Fraction	IC	UC	No	Yes	No	Yes	No	Yes	No	Yes	No		
1	☐. ☐ ☐	5	☐ ☐			☐	☐	☐	☐	☐	☐	☐	☐	
2	☐. ☐ ☐	☐ ☐		☐ ☐		☐	☐	☐	☐	☐	☐	☐	☐	☐
3	☐. ☐ ☐	☐ ☐		☐ ☐		☐	☐	☐	☐	☐	☐	☐	☐	☐
4	☐.☐ ☐	☐ ☐		☐ ☐		☐	☐	☐	☐	☐	☐	☐	☐	☐
5	☐.☐ ☐	☐ ☐		☐ ☐		☐	☐	☐	☐	☐	☐	☐	☐	☐

N.B. Private use is specified by IC 5 Personal/Domestic; This is the direct use of the substance (or a formulation containing the substance) by the public at large.
If the processing step has not to be considered at the assessment “No” is marked (not applicable for IC 5).

4. Production characteristics

D Main producer (tpa): ☐,☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐ Not specified: ☐

IC 3, UC 33

Non-isolated intermediate	(MC 1a)	☐
Isolated intermediate, stored on site	(MC 1b)	☐
Isolated intermediate with controlled transport	(MC 1c)	☐
Not specified	(MC 1c)	☐

Other IC/UC combinations

Continuous production	(MC 1b)	☐
Batch process with dedicated equipment	(MC 1c)	☐
Batch process with multi-purpose equipment	(MC 3)	☐
Not specified	(MC 3)	☐

Production capacity of the main source (producer)

E Capacity (t/day)	☐ ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐
F Period (days/year)	☐ ☐, ☐ ☐ ☐, ☐ ☐ ☐. ☐ ☐ ☐
Not specified	☐

Specific emission information

Emission	**G**: kg/tonne	**or**	Fraction (**EFcomp-prod**)
Air	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Waste water	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Soil	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Not specified	☐		

5. Formulation characteristics

N.B. **For every IC/UC-combination specified in (3) Use and stage of the life cycle:**

∝Specific information on the scale of formulation

One company (fraction of main source = 1)	☐
Fraction of main source (**Fms-form**)	0. ☐ ☐ ☐
specified	☐

∝ No specific emission information

Dedicated equipment and (very) little cleaning operations	(MC 1b)	☐
Dedicated equipment and frequent cleaning operations	(MC 1c)	☐
Multi-purpose equipment	(MC 3)	☐
Unknown		☐

∝ Specific emission information

Emission	**H**: kg/tonne	**or**	Fraction (**EFcomp-form**)
Air	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Waste water	☐ ☐ ☐. ☐ ☐ ☐		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. ☐ ☐ ☐
Waste water	☐ ☐ ☐. ☐ ☐ ☐		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. ☐ ☐ ☐
Waste water	☐ ☐ ☐. ☐ ☐ ☐		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. ☐ ☐ ☐
Waste water	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐
Soil	☐ ☐ ☐. ☐ ☐ ☐		0. ☐ ☐ ☐

Appendix II: Fate of chemicals in a waste water treatment plant based on the SimpleTreat model

The data in Appendix II have been obtained after two modifications to SimpleTreat: one pertaining to the characteristics of the sewage treatment plant, the other implies an improved description of the stripping process. The volume of wastewater is set to 200 instead of 150 l per capita per day. Assuming that the total amount of solids in raw sewage produced per inhabitant per day is still 0.150 ($m^{-3}.d^{-1}$) x 0.6 ($kg.m^{-3}$) = 90 g per inhabitant per day, the concentration of suspended matter in influent has been adjusted to 0.45 ($kg.m^{-3}$) (see Table 7). The hydraulic retention times in the primary settler and the solid liquid separator have not been affected because the volumes (per capita) of these two basins have also been increased by a factor 200/150. Furthermore, in order to maintain the main characteristics of the sludge flow, the steady-state concentration of suspended solids in the primary settler has been reduced by a factor 150/200. It is now 150 mg dry weight per l, implying that still 2/3 of the solids in raw sewage is separated by the primary settler. Consequently, settled sewage flowing from the primary settler into the aeration tank should also contain a reduced oxygen requirement (R_o): (150/200)·235 = 176 mg BOD per l. This correction is necessary as the first order rate constant for stripping of the chemical (when surface aeration is applied) is related to R_o.

A correction for stripping chemicals has been included, as in SimpleTreat the process description is only valid for volatile chemicals (H > 250 $Pa.m^3.mol^{-1}$). The overall mass transfer coefficient during surface aeration (k_{surf}) was assumed proportional to the dissolved oxygen overall transfer rate coefficient ($K_L a_O$), estimated from the oxygen requirement (R_o), hydraulic retention time (HRT) and the difference between the oxygen saturation and the actual O_2 concentration in the aerator (ΔO_2). In order to account also for the gas phase resistance (H < 250 $Pa.m^3.mol^{-1}$) the proportionality constant Ψ, still having the default value of 0.6, should be multiplied by a factor containing the dimensionless Henry constant (K_H) and the ratio of the mass transfer rate coefficients of a chemical in air and water. Munz and Roberts (1987) recommend to apply 40 as a default value for this ratio. As a result the first order rate constant for surface aeration is written as:

$$k_{surf} = \psi \left(\frac{40 \cdot K_H}{40 \cdot K_H + 1}\right) \frac{R_O}{HRT \cdot \Delta O_2}$$

Munz, C.M. and Roberts, P.V. (1989). Gas- and Liquid-Phase Mass Transfer Resistances of Organic Compounds during Mechanical Surface Aeration. Wat. Res. **23**, 589-601.

In the following tables H (Henry's law constant) should be used in $Pa.m^3.mol^{-3}$.

a) No biodegradability

Fate of chemicals that are not degradable: $kbio_{stp}$ = 0 hr^{-1} in the aqueous phase of activated sludge. Operation parameters of the activated sludge reactor: sludge retention time = 7.3 d; hydraulic retention time = 10.4 h; surface aeration.

% to air		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	1	6	47	88	94	95
	1	0	0	0	0	1	6	47	88	94	95
	2	0	0	0	0	1	6	47	88	93	94
log Kow is	3	0	0	0	0	1	5	44	84	90	90
	4	0	0	0	0	0	3	28	61	67	67
	5	0	0	0	0	0	1	6	23	30	30
	6	0	0	0	0	0	0	1	4	7	8

% to water		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	100	100	100	100	99	94	53	12	6	5
	1	100	100	100	100	99	94	53	12	6	5
	2	99	99	99	99	99	94	53	12	6	5
log Kow	3	93	93	93	93	92	88	50	12	6	5
	4	56	56	56	56	56	53	34	9	5	4
	5	15	15	15	15	15	14	12	6	4	4
	6	7	7	7	7	7	7	7	6	5	5

% to sludge		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
log Kow	3	7	7	7	7	7	7	6	5	4	4
	4	44	44	44	44	44	44	38	30	28	28
	5	85	85	85	85	85	85	82	71	66	66
	6	93	93	93	93	93	93	92	90	87	87

% removal		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	1	6	47	88	94	95
	1	0	0	0	0	1	6	47	88	94	95
	2	1	1	1	1	1	6	47	88	94	95
log Kow	3	7	7	7	7	8	12	50	88	94	95
	4	44	44	44	44	44	47	66	91	95	96
	5	85	85	85	85	85	86	88	94	96	96
	6	93	93	93	93	93	93	93	94	95	95

b) Inherent biodegradability

Fate of chemicals that are "inherently biodegradable" in an OECD/EU test: $kbio_{stp}$ = 0.1 hr^{-1} in the aqueous phase of activated sludge. Operation parameters of the activated sludge reactor: sludge retention time = 7.3 d; hydraulic retention time = 10.4 h; surface aeration.

% to air		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	0	3	30	77	88	89
	1	0	0	0	0	0	3	30	77	88	89
	2	0	0	0	0	0	3	30	77	87	89
log Kow	3	0	0	0	0	0	3	29	74	84	85
	4	0	0	0	0	0	2	19	54	63	64
	5	0	0	0	0	0	0	5	21	28	29
	6	0	0	0	0	0	0	1	4	7	7

% to water		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	49	49	49	49	49	47	33	11	6	5
	1	49	49	49	49	49	47	33	11	6	5
	2	49	49	49	49	48	46	33	10	6	5
log Kow	3	46	46	46	46	46	44	31	10	5	5
	4	32	32	32	32	32	31	23	8	5	4
	5	12	12	12	12	12	12	10	6	4	4
	6	7	7	7	7	7	7	7	6	5	5

% to sludge		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
log Kow	3	6	6	6	6	6	6	5	5	4	4
	4	37	37	37	37	37	36	34	29	28	28
	5	81	81	81	81	81	81	78	70	66	65
	6	92	92	92	92	92	92	92	89	87	87

% degraded		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	51	51	51	51	51	50	37	12	7	6
	1	51	51	51	51	51	50	37	12	7	6
	2	51	51	51	51	51	50	37	12	6	6
log Kow	3	48	48	48	48	48	47	35	12	6	6
	4	31	31	31	31	31	31	24	8	5	4
	5	7	7	7	7	7	7	6	3	2	2
	6	1	1	1	1	1	1	1	1	1	1

% removal		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	51	51	51	51	51	53	67	89	94	95
	1	51	51	51	51	51	53	67	89	94	95
	2	51	51	51	51	52	54	67	90	94	95
log Kow	3	54	54	54	54	54	56	69	90	95	95
	4	68	68	68	68	68	69	77	92	95	96
	5	88	88	88	88	88	88	90	94	96	96
	6	93	93	93	93	93	93	93	94	95	95

c) pass levels within 28 days in a test on "ready biodegradability", 10 day window criterion is not fulfilled
Fate of chemicals that reach the biodegradation pass levels within 28 days in an OECD/EU test on "ready biodegradability but not within the 10 day time window: $kbio_{stp}$ = 0.3 hr^{-1} in the aqueous phase of activated sludge. Operation parameters of the activated sludge reactor: sludge retention time = 7.3 d; hydraulic retention time = 10.4 h; surface aeration.

		log H									
% to air		-4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	0	2	18	63	78	80
	1	0	0	0	0	0	2	18	63	78	80
	2	0	0	0	0	0	2	18	62	77	79
log Kow	3	0	0	0	0	0	2	18	60	74	76
	4	0	0	0	0	0	1	12	44	56	57
	5	0	0	0	0	0	0	4	18	25	26
	6	0	0	0	0	0	0	1	4	7	7

		log H									
% to water		-4	-3	-2	-1	0	1	2	3	4	5
	0	24	24	24	24	24	23	19	8	5	5
	1	24	24	24	24	24	23	19	8	5	5
	2	24	24	24	24	24	23	19	8	5	5
log Kow	3	23	23	23	23	23	22	18	8	5	4
	4	17	17	17	17	17	17	14	7	4	4
	5	9	9	9	9	9	9	8	5	4	3
	6	7	7	7	7	7	6	6	6	5	5

		log H									
% to sludge		-4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	1	1	1	1	1	1	1	0	0	0
log Kow	3	5	5	5	5	5	5	5	4	4	4
	4	32	32	32	32	32	32	31	29	28	28
	5	75	75	75	75	75	75	74	68	65	65
	6	91	91	91	91	91	91	91	89	87	86

		log H									
% degraded		-4	-3	-2	-1	0	1	2	3	4	5
	0	76	76	76	76	76	75	63	29	17	16
	1	76	76	76	76	76	75	63	29	17	16
	2	75	75	75	75	75	74	63	29	17	16
log Kow	3	72	72	72	72	72	71	60	28	16	15
	4	50	50	50	50	50	50	43	21	12	11
	5	16	16	16	16	16	16	14	9	6	5
	6	2	2	2	2	2	2	2	2	2	1

% removal		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	76	76	76	76	76	77	81	92	95	95
	1	76	76	76	76	76	77	81	92	95	95
	2	76	76	76	76	76	77	81	92	95	95
log Kow	3	77	77	77	77	77	78	82	92	95	96
	4	83	83	83	83	83	83	86	93	96	96
	5	91	91	91	91	91	91	92	95	96	97
	6	93	93	93	93	93	94	94	94	95	95

d) pass levels within 28 days in a test on "ready biodegradability", 10 day window criterion is fulfilled
Fate of chemicals that are "readily biodegradable" in an OECD/EU test: $kbio_{stp}$ = 1 hr^{-1} in the aqueous phase of activated sludge. Operation parameters of the activated sludge reactor: sludge retention time = 7.3 d; hydraulic retention time = 10.4 h; surface aeration.

% to air		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	0	2	9	38	56	59
	1	0	0	0	0	0	2	9	38	56	59
	2	0	0	0	0	0	1	9	38	56	58
log Kow	3	0	0	0	0	0	1	9	37	53	56
	4	0	0	0	0	0	1	6	27	40	42
	5	0	0	0	0	0	0	2	12	19	20
	6	0	0	0	0	0	0	0	3	6	6

% to water		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	9	9	9	9	9	8	7	5	4	3
	1	9	9	9	9	9	8	7	5	4	3
	2	9	9	9	9	9	8	7	5	4	3
log Kow	3	8	8	8	8	8	8	7	5	3	3
	4	7	7	7	7	7	6	6	4	3	3
	5	5	5	5	5	5	5	5	4	3	3
	6	6	6	6	6	6	6	6	5	5	5

% to sludge		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	0	0	0	0	0
	2	0	0	0	0	0	0	0	0	0	0
log Kow	3	4	4	4	4	4	4	4	4	4	4
	4	29	29	29	29	29	29	29	28	28	28
	5	68	68	68	68	68	68	67	65	64	64
	6	88	88	88	88	88	88	88	87	85	85

% degraded		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	91	91	91	91	91	90	84	57	41	38
	1	91	91	91	91	91	90	83	57	41	38
	2	91	91	91	91	91	90	83	57	40	38
log Kow	3	87	87	87	87	87	86	80	54	39	36
	4	64	64	64	64	64	64	59	41	29	28
	5	27	27	27	27	27	27	26	19	14	14
	6	6	6	6	6	6	6	6	5	4	4

% removal		log H -4	-3	-2	-1	0	1	2	3	4	5
	0	91	91	91	91	91	92	93	95	96	97
	1	91	91	91	91	91	92	93	95	96	97
	2	91	91	91	91	91	92	93	95	96	97
log Kow	3	92	92	92	92	92	92	93	95	97	97
	4	93	93	93	93	93	94	94	96	97	97
	5	95	95	95	95	95	95	95	96	97	97
	6	94	94	94	94	94	94	94	95	95	95

Appendix III: Evaluation of data

In determining whether or not the data to be used in the risk assessment are adequate, their quality and representativeness needs to be evaluated. For this, a number of factors will be considered and the test design will be evaluated to ensure that the quality criteria demanded by standardised tests have in part or in whole been met. Such quality criteria can be detailed in general terms but expert judgement will be required for each substance and test data on a case-by-case basis.
A number of papers address the issue of data quality (e.g. SIDS Manual (OECD 1994a); AQUIRE-database-manual; Tema Nord, 1994). Care should be taken that the guidance given is appropriate for the use of data.
The following factors should be taken into account when evaluating the data (on aquatic toxicity):

1. Identity of the test substance

It is important that the substance tested be properly identified and any significant impurities described. Ideally, this should be through the quoting of a CAS No. or other substance specific means but the substance name may often be sufficient. However, tests conducted on 'dichloro.....' when the substance being evaluated is '1,3-dichloro.....' may thus be insufficient to determine exactly what substance was tested. Equally, the presence or absence of a significant toxic impurity may affect the measured toxicity. Where such an impurity is identified in the substance under evaluation, due care should be taken to ensure that its effects are fully taken into account.

2. Test organisms

Detailed information of the taxonomic identity of aquatic organisms tested should be supplied, to include the genus and species. While tests on 'non-standard' organisms can be accepted, care should be taken to ensure that they are properly characterised and the test system appropriate. The animals should be of relatively uniform age, weight and size and should be healthy at the start of test as shown by low mortality/effects in controls.

3. Test design

The test system should be adequately described and be considered appropriate for the substance of concern and organisms tested. The delivery of the test substance should be ensure a controlled and known exposure and the supply of oxygen, food and light be suitable to reduce unnecessary stress in the test organisms. The temperature, pH and water hardness should be recorded and be appropriate for the organisms tested. The number of organisms exposed and number of exposure concentrations chosen should be sufficient for a valid statistical calculation of the appropriate effects concentrations to be made.

- The delivery of the test substance represents a critical stage in ensuring adequate exposure of the test organisms. When considering the delivery system, due account should be taken of the relevant phys. chem. properties of the test substance and their potential effects on the delivery and exposure systems. For Daphnia and algae static tests are normally used but for fish static, semi-static or flow-through tests may be appropriate. The precise mechanism used to deliver the test substance must therefore be described;

- The exposure concentration should be known and maintained under control (>80% of initial concentrations) throughout the test. Ideally, the concentrations should be directly measured at appropriate stages over the course of the test. In many cases, measured concentrations will not be available and expert judgement will be necessary to decide whether the exposure of the aquatic organisms is adequately described. Such non-measured concentrations are normally described as 'nominal' concentrations and refer to the level at which it was intended that exposure would occur. Such concentrations may be acceptable if the test substance:
  - is sufficient soluble in test water, i.e. the test concentrations are below the water solubility;
  - is relatively stable in test water;
  - has a low absorbance to the system delivery and exposure apparatus;
  - is non-volatile.

  For the interpretation of data that were generated by using solubilisers the altered bioavailability (enhancement/reduction) has to be considered. For many substances, including poorly water soluble substances, volatile substances and substances that hydrolyse or adsorb on surfaces, nominal concentrations are often not appropriate and additional information may be necessary in order to verify the actual exposure concentrations. In some cases, the choice of a semi-static or flow-through system (fish test) may allow a presumption of a stable exposure concentration. In general, the more likely it is that the physical chemical properties of the substance would lead to a loss of concentration over the course of the test, the more important it becomes to verify the concentration by direct analysis of the test water at suitable points throughout the test. Where the exposure concentration can not be determined with confidence, the test should be regarded as ' not-valid' for the purposes or risk assessment;

- The environmental conditions which exist during the test should be recorded and be both stable and appropriate. Significant variations in the environmental conditions such as pH, temperature, water hardness, oxygen levels and light regime can induce undue stress within the test organisms and hence false levels of toxicity. Absence of information on these parameters would suggest that the test system was not well described although would not necessary invalidate the data if other quality criteria are met;

- The L(E)C50 would normally be determined on a statistical basis from the effects observed over a range of concentrations. It is important, therefore, that sufficient organisms are tested at each concentration level and sufficient concentration levels are chosen so as to allow a statistically valid derivation to be made of the appropriate effect concentration. In the absence of this details, a clear indication of the method used to calculate the effect (or no effect) concentration may be sufficient. Limit tests would not normally be acceptable expect as a means of demonstrating no toxic effects;

- At issue is whether the duration of a standard toxicity test(s) is long enough for the compound to reach steady state and elicit a toxic response (Hawker and Connell, 1985; Connell, 1990; Kristensen and Tyle 1990). For many organic non-metabolizable compounds, the time to reach respectively 80% and 95% of the steady state concentration is depending on lipophilicity of the compound (OECD, 1994b).

4. Field studies

In general field studies are difficult to interpret. Touart (1988) developed guidance criteria for aquatic mesocosm tests with pesticides. Emans et al. (1993) used a set of criteria to assess the quality of field studies. This set can serve as a tool for evaluation:

1. a distinct concentration-effect relationship should be obtained,

2. a reliable MS NOEC should be derived,

3. several taxonomic groups, in more or less natural ecosystems, should be exposed to one test concentration for a longer period,

4. in each experiment several concentrations should be tested, consisting of one control and at least two test concentrations,

5. each test concentration should have at least one replica,

6. the concentration of the test compound should be measured several times during the experiment,

7. physico-chemical parameters like pH, temperature and hardness should be measured,

8. apart from effect parameters like population density and biomass also effect parameters on higher integration levels such as species diversity and species richness should be measured.

5. References

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Appendix IV: Assignment of organisms to trophic levels

Primary producers

Primary producers photo-/chemo-autotrophically synthesise organic compounds using inorganic precursors. They include:

- chlorophyll-containing species of vascular plants
- algae, (e.g. green algae: *Selenastrum*, *Scenedesmus*, *Chlorella*; blue-green algae: *Microcystis*)
- purple sulphur bacteria, chlorobacteria
- chemoautotrophic bacteria (nitrifying bacteria, sulphur bacteria).

Primary consumers

They live mainly on living or dead autotrophic organisms or on microorganisms. Representatives of this trophic level are especially plant-eating animals (i.e. species that are not carnivorous of the following taxonomic groups):

- protozoa (e.g. *Uronema, Entosiphon, Tetrahymena*)
- annelida (e.g. *Tubifex, Enchytraeus*)
- crustacea (e.g. *Artemia, Daphnia* spec., *Copepoda, Gammarus, Asellus*)
- molluscs (e.g. *Dreissena, Mytilus, Ostrea*; several gastropods: *Patella, Viviparus*)
- insects (some insect larvae that are not carnivorous)
- nematoda (those species which are living in water)

Secondary consumers

They live mainly on primary consumers. Among them are:

- predatory insects and larvae of insects (e.g. *Chaoborus*)
- carnivorous protozoa
- rotatoria
- coelenterata (e.g. *Hydra*)
- predatory copepods
- fish (*Teleostei*: e.g. *Cyprinus carpio*, *Brachydanio rerio*, *Poecilia reticulata*, *Oryzias latipes*, *Pimephales promelas*, *Lepomis macrochirus*, *Oncorhynchus mykiss* (previously: *Salmo gairdneri*, *Leuciscus idus melanotus*, *Cyprinodon, Carassius*)
- amphibians (e.g. *Rana, Xenopus*)

Decomposers

Organisms of this trophic level break down dead organic material to inorganic 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 reason for their sensitivity to a certain toxic chemical.

The standard organisms which are usually used in standard tests (plankton micro-algae, Daphnia and fish) represent three trophic levels (primary producers, primary consumers and secondary consumers), three taxonomic groups (green algae, crustaceans and bone fish), two life forms (plankton or nekton) and three feeding strategies (photosynthetic, herbivorous filter feeder and carnivorous).

Accordingly, non-standard organisms can be assigned to equivalent trophic levels, taxonomic groups etc.

The assignment of an organism to a trophic level is based on the energy balance of the ecosystem concerned and is not primarily dependent on the species. Therefore, a given population may represent more than one trophic level depending on the spectrum and amount of nutrition for the species. In addition, earlier life stages may live on completely different nutrition compared to adults of the same species.

Appendix V: Statistical extrapolation method

The effect assessment performed with assessment factors can be supported by a statistical extrapolation method if the data base is sufficient for its application. If a large data set from long-term tests for different taxonomic groups is available (OECD, 1992) statistical extrapolation methods may be used to derive a PNEC. The use of identical parameters (e. g. reproduction) for the determination of the NOECs is still being discussed. Identical parameters are suggested by Van Straalen and Dennemann (1989) and especially if only limited data from different species are available also by Løkke (1994).

Main underlying assumptions of the statistical extrapolation methods are the following (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. Until now, most authors have set this percentile at 95 % (OECD, 1992). This means that the NOEC may be exceeded for 5 % of the species of the community. The 95 % protection level may be regarded as a 'politically' fixed value (Løkke, 1994).

Several distribution functions have been proposed. The 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 validity of several of the assumptions mentioned above are still subject of scientific discussion (Løkke, 1994; Forbes and Forbes, 1993). First of all, the distribution model was used. As for most compounds, few long-term NOECs are available most tests of the shape of the distribution have low power. Secondly, it is obvious that the NOECs available are not a random sample. Wagner and Løkke (1991) argued that it is more important to have a selection of species that are representative of the ecosystem.

The approach of statistical extrapolation is still under debate and needs further validation. An advantage of these methods is that they use the whole sensitivity distribution of species in an ecosystem to derive a PNEC instead of taking always the lowest long-term NOEC. A first validation of these methods was carried out by Emans et al. (1993) who compared results from aquatic multi-species tests with statistical extrapolation methods and methods using assessment factors. They concluded that statistical extrapolation methods seem to be a good basis for deriving 'safe' values for aquatic ecosystems.

Summarising, it is recommended to use statistical extrapolation methods as a supplementary approach. If more experience is gained with these methods and they are validated to a larger extent, in the future PNECs derived by these methods may be used instead of PNECs derived by assessment factors. However, if these methods are used the assumptions, e.g. the distribution model, must be checked. As the outcome of the different methods are almost equal (OECD, 1992; Emans et al., 1993) all methods can be used: triangular, log-logistic or log-normal distribution.

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Appendix VI: Examples of assays suitable for further testing for soil and sediment organisms

1. Soil organisms

In table 1 tests with soil organisms are presented

Table 1 *Toxicity tests with soil organisms*

Standardised tests (guidelines or draft guidelines) Tests on organisms: Effects on microorganisms 1)2)3) Modification: use of European "standard soils": Parameter: nitrification soil respiration dehydrogenase, unrease and phosphatase activity Long-term test on earthworms 1) Parameter: reproduction Long-term test on Collembola: Parameter: reproduction	Methods e. g. published by: Denmark, Netherlands, Germany - BBA VI, 1-1 (1990a) ISO Draft (1993), Netherlands Netherlands, Germany-BBA Draft (1990b)
Semi-standardised tests: (e. g. international ring tests are necessary) Tests on organisms Coleoptera-Tests e.g. Long-term test on Staphylinidae Parameter: degree of paratism, hatching or reproduction Long-term test on Enchytraeus Parameter: reproduction (as alternative to a reproduction-test with earthworms)	 Methods e. g. published by: Samsoe-Petersen (1987), Naton (1989), SETAC (1995) Draft guideline Römbke (1991)

1) In case this test was not available for the initial risk characterisation.
2) Problems of the use of this test are discussed by Stavola (1990).
3) Guidelines developed for testing of pesticides.

A few species that belong to additional taxonomic groups and are suitable test organism were indicated in the SERAS-Workshop in 1992 (Soil Ecotoxicological Risk Assessment System). Van Straalen and Van Gestel (1992), Stavola (1990) and Pedersen and Samsoe-Petersen (1993) discuss a number of terrestrial species and test methods with various degrees of standardisation. Léon and Van Gestel (1994) give possible criteria for the evaluation of individual tests and for the selection of standardised laboratory toxicity tests with terrestrial organisms.

It should be considered that the results obtained by tests according to the guidelines for pesticides pose a similar problem. Only tests where the test substance is applied to the soil in a comparable way to the exposure of existing chemicals can be used for the concentration-effect assessment. After recognising the lack of standardised soil tests, research programmes have been initiated in Sweden (MATS = MArk Test System), in the Netherlands (NISRP = Netherlands Integrated Soil Research Programme) and in Denmark.
Recently, also a coordinated development and standardisation of a number of test species and test systems for an ecotoxicological approach has been initiated. This project SECOFASE (Sublethal Effects of Chemicals On FAuna Soil Ecosystem) is described by Løkke and Van Gestel (1993, cited in Pedersen and Samsøe-Petersen (1993)). It should be mentioned that the guideline for a long-term test with vascular plants has still to be finalised (e.g. with *Arabidopsis thaliana* or *Brassica rapa*, Stavola (1990)). Long-term tests for the earthworm (ISO draft, 1993; Dutch Draft Guideline; German Draft Guideline) and the spring-tail (Dutch Draft Guideline; German Draft; BBA 1990b) are available. Both tests analyse effects on reproduction. In addition, the standardisation of the following two long-term tests is close to completion: the test on Staphylinids (*Coleoptera*) where degree of parasitism, hatching rate and reproduction are registered (Samsoe-Petersen, 1987; Naton, 1989; SETAC, 1995) and the test on Enchytraea (*Annelidae*) which can be used instead of the reproduction tests on earthworms (Römbke, 1991).

2. Sediment organisms

In table 2 sediment tests which are used in the United States are listed (Burton, 1991). Organisms which depend on the sediment as well as organisms which depend on the water layer above the sediment are presented.

Table 2 *Toxicity tests with sediment organisms*

Biological group/Test organism	**Parameter tested**
Benthic invertebrates	
nematodes:	
Panagrellus redivivus	survival
Caenorhabditis elegans	survival
oligochaetes:	
Tubifex tubifex	survival
Stylodrilus heringianus	survival, repellency, rate of transformation of the sediment, growth
amphipods:	
Hyalella azteca	survival, growth, reproduction
Pontoporeia hoyi (Diporeia sp.)	survival, repellency
Corbicula fluminea	survival, growth
pelecypods:	
Anodonata imbecilis	survival
insects:	
Chironomus tentans	survival, growth, hatching
Chironomus riparius	survival, growth
Hexagenia limbata	survival, frequency of exuviation
macrobenthic biocoenoses	indices for biocoenoses and populations
macrophytes:	
Hydrolla verticilata	length of shoots and roots, dehydrogenase activity, chlorophyll a, peroxidases

3. References

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Appendix VII: Toxicity data for fish-eating birds and mammals

The endpoints of the tests should be expressed as a concentration in food (mg test substance/kg food). Often test results for birds and mammals are expressed in mg/kg body weight/day. These data should be converted to a concentration in food (mg/kg). For the conversion, data on body weight and daily food intake during the tests need to be known. This conversion is only advisable when no other toxicity data for birds and mammals are available. If this information cannot be obtained from the test report, the values on body weight, daily food intake and daily water intake that are given in the table can be used for the transformation. For transformation of toxicity data expressed on the basis of body weight or water intake to food intake, the toxicity data should be multiplied by the conversion factor (BW/DFI or DWI/DFI).

Table 1 *Conversion factors for toxicity data (Sax, 1989; Romijn et al., 1993)*

	BW	DFI	DWI	BW/DFI	DWI/DFI
Canis domesticus	10,000	250		40	
Macaca spec.	5,000	250		20	
Microtus spec.	25	3		8.3	
Mus musculus	25	3		8.3	
Oryctolagus cuniculus	2,000	60		33.3	
Rattus norvegicus (> 6 weeks old)	200	10		20	
Rattus norvegicus (< 6 weeks old)				10	
Gallus domesticus		64.3	128.5		2

BW : body weight (g)
DFI : daily food intake (g/day)
DWI : daily water intake (mg/l/day)
BW/DFI : conversion factor from mg/kg body weight/day to mg/kg food
DWI/DFI : conversion factor from mg/l/day to mg/kg food

Concentrations causing no effect after long-term exposure (NOEC) are preferred. If, in a study, a single dose or the lowest dose of a range causes < 20 % mortality, a NOEC may be calculated from LOEC/2. If the effect is more than 20 %, the data cannot be used.
Laboratory food for mammals and birds is usually grain. The energy content of grain is higher than fish. This means that in order to obtain the same amount of energy more wet weight of fish must be consumed compared to grain. Therefore a correction factor of 3 may be applied for the difference in caloric content of the diet of laboratory animals and the diet of fish-eating birds or mammals (Everts et al., 1993).

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Appendix VIII: Environmental risk assessment for metals and metal compounds

1. Introduction

This document gives a general outline on how to perform risk assessments for metals using the methods that are available for risk assessment of new and existing organic chemicals as a starting point. There are a number of fundamental differences between metals and organic chemicals that must be taken into account when assessing the risks to man and the environment, e.g.

- Unlike most organic chemicals, metals, and a limited number of organometallo compounds like methylmercury and methyltin, are a class of chemicals of natural origin. Consequently natural background concentrations and the exposure due to these background concentrations should be taken into account during risk assessment;
- The availability of metals for uptake by organisms under field conditions is limited, will vary from site to site and is highly dependent on the speciation of the metal. Hence, it is of utmost importance that both PEC and PNEC are based on similar levels of availability in both exposure and effect assessment, taking the speciation into account;
- The same toxic form can originate from a variety of different substances, e.g. Zn^{2+} from $ZnSO_4$, $ZnCl_2$ etc. Therefore it is in general necessary to take into account all metal species that are emitted to the environment which in the end lead to concentrations of the toxic form.

Substantial levels of information are available regarding the fate and toxicity of metal ions and this information will be examined to improve the assessment process. However, it is recognised that many of the specific fate and toxicity extrapolations are either not appropriate or need modification. The interaction of metal ions with the media in both the aquatic and soil compartments may result in a high level of uncertainty regarding the true level of bioavailablity of the toxic species necessary for a practical assessment.

Organo-metallic compounds are not explicitly covered by this procedure unless they act, through their degradation products, as significant sources of the toxic metal ion. It is considered that these organo-metallic compounds can generally be assessed as individual substances in accordance with the procedures laid down in the main text (Chapter 3). When the emissions of these substances are major contributors to the toxic metal ion concentration in either a local or regional environment, they will be further assessed according to the procedures laid down in this document.

When describing the topics that need to be taken into consideration for the risk assessment of metals, there is often a misunderstanding with regard to definitions of some of the key terms. In this appendix the following definitions will be used for these key terms:

General:

- **total concentration of a metal**: for terrestrial systems, the concentration of a metal that is determined after complete destruction of the mineral matrix. For aqueous systems: the total amount of metal present, including the fraction sorbed to particles and to dissolved organic matter and the fraction in the mineral matrix;
- **available fraction**: the fraction of the metal that is extractable from the substrate with chemical (e.g.: neutral salt, water extraction) or physical means (shaking, pore water collection), and that is generally considered to be a better estimate for the fraction that is potentially available for organisms than the total concentration;
- **bioavailable fraction**: the fraction that is available for uptake by a specific organism. A single substrate has only one 'availability' for each of the possible physico-chemical extraction procedures. The bioavailability differs, however, per biological species. Thus, taking soil as an example, for instance for worms in a certain soil the bioavailability may be high (it is in this case the concentration in the pore water that determines uptake), while for arthropods in the same soil the bioavailability may be low (uptake by the food is for these organisms the dominant uptake route);
- **natural background concentration**: the concentration that is present due to natural causes only;
- **ambient background concentration**: the concentration that is present due to natural background plus the immission of metals from diffuse sources of human origin[1].

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;

1 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 * (L + H) ; [Zn] = 50 + 1.5 * (2L + H) or [Ni] = 10 + L.

- **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).

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, 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. New substances, for example, must be assessed for their impact following local emissions. In general their contribution to the larger environmental burden will be small until high annual tonnages are reached.

2.1 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 waste water treatment plant can be modelled using SIMPLETREAT, although measured K_p values will have to be used (section 2.3.7 of main text). Since the actual bioavailability of the metal ion will be determined by the properties of the receiving media, such as the pH and water hardness, the precise physico-chemical characteristics of this receiving media must be defined. In general, it will be defined in a way which optimises the bioavailability of the toxic species. Speciation models exist which may be used to determine the soluble fraction. The partitioning behaviour of the substance to sludge/sediment/soil can be based on the appropriate 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.

2.2 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 the main text). The same applies to the bioconcentration factors required: only experimentally determined values should be used (see section 3.8 of the main text and section 3.3 of this appendix). For soils, the 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 1.
In general, the mathematical descriptions of fate processes used in multimedia fate models are also applicable to local models.

2.3 Background concentrations

When assessing the exposure of man and ecosystems to metals previous releases into the environment need to be considered. In view of differences in bioavailability (see below) it is important to distinguish between ambient background concentrations and natural background concentrations. One should be aware that natural background concentrations within an environmental compartment may vary from site to site by several orders of magnitude. Also, due to natural dynamic processes like weathering, natural background concentrations may change over time. This means that it is impossible to attribute single values to natural background concentrations of specific metals within a certain compartment. It should be noted that under natural conditions in certain regions, clearly elevated natural background concentrations can be encountered. When assessing the natural background concentration within a certain area, these 'outliers' should not be used or included in the calculation of the standard background concentrations as they would give a non-representative picture thereof.

Several methods are available for determining background concentrations. Apart from the obvious method of measuring metal levels at selected sites considered to be undisturbed by human activities, additional methods include:

- Geochemical modelling: estimation methods on the basis of the contribution of weathering processes (erosion). This method is shown to be well applicable for assessing natural background concentration in aqueous systems (rivers).
- Assessment of metal concentrations in the deeper sediment layers, taking into account anthropogenic contributions and leaching to these layers.
- For surface water having ground water as its origin: assessment of the metal concentrations in the deeper ground water.

For soils, ambient background concentrations can be calculated as described above (reference lines). Through this procedure the natural binding capacity of soils, making the metal more or less inert in the solid phase, is approximated. Application of this procedure to both laboratory toxicity data and to field soils is possible.

For surface water extensive national monitoring programs exist for the follow-up of metals in the aquatic environment since most metals are considered in the EC Regulation 76/464 as list I ("black list") or list II ("grey list") substances. Extraction of representative natural background concentrations may be possible from these data. However, these monitoring programs often measure total instead of dissolved metal concentrations.

2.4. 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.

Multimedia fate models can be used to estimate exposure to metals. However, there are several differences compared to the use of these models for organic compounds. Below, differences are described for applying regional models. Reference is made to the sections in the main text.

1. Physico-chemical properties (section 2.3.2)
In general water solubility, boiling point and vapour pressure cannot be used. The octanol-water partitioning coefficient is not appropriate and measured partition coefficients K_p should be used instead.

2. Partition coefficients (section 2.3.5)
Adsorption to aerosol particles
Most of the metal present in the atmosphere will be bound to aerosols. Therefore, an extremely low value for the vapour pressure should be used in formula 5 on page 31, e.g. 10^{-20} Pa. This leads to a value for $Fass_{aer}$ almost equal to one. If a valid measured value is available, this value can be used.

Volatilisation
Volatilisation can be ignored for metals, except for mercury-compounds and several organometallo compounds. Therefore the Henry-coefficient should be set to a very low value (formula 6).

Adsorption/desorption
Formula 8 and 9 cannot be used. As stated in this appendix, measured K_p values must be used for water-soil, water-sediment and water-suspended matter.

3. Biotic and abiotic degradation rates (section 2.3.6)
Not important for regional models.

4. Elimation processes prior to the release in the environment (section 2.3.7)
For applying models like SimpleTreat a partition coefficient is used for water-sludge. For metals a measured K_p value must be used. However, it should be noted that K_p values are different for the different metal species.

5. Calculation of $PEC_{regional}$ (section 2.3.8.7)
The values applied for model parameters for the regional model (Table 10), intermedia mass transfer coefficients (Table 11) and model parameters for the continental concentration (Table 12) can be used.

***Figure 1**: Use of multimedia fate models for metals*

In a natural soil or sediment system, metals can be distributed over the following fractions:

- dissolved in the pore water,
- reversibly or irreversibly bound to soil or sediment particles,
- reversibly or irreversibly bound to organic ligands,
- encapsuled in secondary clay minerals and metal(hydr)oxides,
- encapsuled in the primary minerals.

It is recognised that for various organisms, only the metal species present in the aqueous phase (pore water) are potentially available for direct uptake by biota and thus mainly responsible for effects on biota. Other uptake routes may also be important, especially for metals with high 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:

$$K_p = \frac{\textit{total available concentration in solid phase}}{\textit{concentration in aqueous phase}} \qquad (1)$$

It is of importance to be aware that equation 1 differs from the commonly used expressions for 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 (1). However, up till now the underlying concepts for a standardised approach towards partition coefficients representing availability have not yet been sufficiently worked out.

Finally, with regard to availability of metals it should be noted that apart from the general processes denoted above, under certain environmental conditions additional complexation and precipitation processes may take place that may strongly diminish aqueous metal concentrations. An example of such a process is the formation of insoluble metalsulphides under anaerobic conditions (the so-called Acid Volatile Sulphide, or AVS-concept).

2.5. 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.

3. Effects assessment

3.1. Availability of data

Toxicity data are available for most metals in sufficient quantity, since there are few compounds, and various toxicity data exist at least for the soluble metal salts. Most data are available for the toxic effects of metals on aquatic organisms, to a lesser extent data are present for terrestrial and sediment-dwelling organisms. Usually most data are based on total concentrations of the metals under investigation. For essential metals deficiency data must be taken into account.

The data are available both on short and long term tests, and are present for species from various trophic levels. These data can be used for the effect assessment in all compartments following the procedures for assessing the adequacy of data as presented in the main text (see section 3.2). However, some metal-specific criteria must be taken into account:

- physico-chemical test conditions that define the metal speciation and bioavailability should be relevant for field conditions: water hardness, pH, alkalinity, presence of complexing agents (humic acids and EDTA);
- content of metal already present in the test medium, especially for soils taken from the field and natural waters. As metals are natural constituents of the biosphere these background concentrations can influence the test results. However, it should be noted that the bioavailability of the background concentration for soils is probably less than that of the "added" metal;
- for essential metals organisms of a given habitat are conditioned to the natural concentration range for essential elements. Within this range they can regulate their metal uptake in such a way that their internal concentration is kept relatively stable (homeostasis). This implies that organisms tested should originate and be cultivated within this optimal concentration range.

3.2. Derivation of the PNEC

PNECs can be derived through the application of assessment factors on the basis of the available data assessed according to the criteria given above. Standard methods applied elsewhere (e.g. for organic compounds) can be used for this (see sections 3.3/3.7 of the main text). However, because of the specific mode of action that metals may have for some species, care should be taken in extrapolating short term toxicity data to the PNEC using the standard assessment factors in section 3.3. For many metals sufficient long term toxicity data for aquatic organisms may be present to enable statistical extrapolation, results of which can support the results of PNECs calculated using assessment factors.
Calculated PNECs derived for essential metals may not be lower than natural background concentrations.

A prerequisite for the derivation of the PNEC is that it is done on the basis of the same level of availability as in exposure assessment:

- Results from aquatic toxicity tests are usually expressed as total concentrations. As a first approach total concentrations have to be recalculated to dissolved concentrations using partition coefficients. If this is not possible, the total concentration can be set equal to the dissolved concentration. Differences in test systems, e.g. (semi-)static versus continuous flow systems and natural versus standard water, have to be considered;
- For the terrestrial compartment many data exist, but most are only expressed as total concentration that has been added to the test media. This added amount will be partitioned among the aqueous and the solid phase. Application of partition coefficients to calculate the available concentration in soil can be applied. Soil type correction, using reference lines should be applied to correct for differences among soil types (see also section 3.6.2 of the main text).

In future risk assessment for the terrestrial compartment one should be aware of the different routes of exposure that exist among terrestrial species: for species that are not exposed through the aqueous phase, the (physico-chemically) available fraction needs not be correlated to the bioavailability;

- Some of the metals are essential metals, having a function in biological processes at low concentrations. Shortage of micronutrients may cause malfunction. This implies that in setting the PNEC information on deficiency levels should be taken into account. It should, however, be noted that often no information on deficiency levels of various metals for various species is available.

Though some exceptions exist, in general ionic metal species are considered to be the dominant metal species taken up, and are thus considered to be the metal species responsible for the toxic effect. Data on the concentration of ionic species in aquatic and terrestrial systems are not readily available, and cannot, as yet, be applied on a regular basis in risk assessment.

3.3 Bioaccumulation of essential metals

Metals are taken up by organisms. For essential metals, biota regulate their uptake by means of the general physiological mechanism of homeostasis. By this mechanism, organisms will keep within a certain range of varying external concentrations, their intracellular levels relatively constant, in order to satisfy their requirements for that essential element. Homeostasis implies that organisms can deliberately concentrate essential elements if concentrations in the environment are very low. This may lead to high BCF values. On the other hand, the homeostatic regulation capacity will be exceeded at a given higher external concentration beyond which the element will accumulate and become toxic.

4. Risk Characterisation

The risk characterisation of metals basically follows the principles set out in section 4 of the main text. However, it should be stated again that is very important that both PEC and PNEC are based on similar levels of availability. In addition, when PEC/PNEC ratios greater than one are found, it is very important to have information on the natural and/or ambient background levels in order to decide upon further actions to be taken to reduce the risks.

Since for most metals sufficient monitoring data are obtainable, risk assessment will often be based on measured instead of calculated environmental concentrations, especially for a regional assessment. Usually most monitoring data deal with total concentrations. Especially in case of aqueous systems it often is well possible to convert measured total concentrations to dissolved concentrations. For terrestrial systems this is possible by applying the appropriate K_p-values.

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Appendix IX: Environmental risk assessment for petroleum substances

1. Introduction

In the present appendix the Hydrocarbon Block Method (HBM) is described, which is under development and may be used for environmental risk assessment of petroleum substances. The method was originally devised by CONCAWE (The Oil Companies' European Organisation for Environmental and Health Protection) and was discussed in a workshop in Ispra in December 1994 (CONCAWE, 1995; EU, 1995). The approach has only recently been devised and hence experience with its application is limited. Although there has been work to validate the general approach, it should be recognised that there are still uncertainties regarding some technical details which should be borne in mind, when considering the outcome of the risk characterisation.

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", be they single or multiple component "blocks". These blocks should show similar modes of action.
From the above it is clear that the PEC/PNEC ratio of the whole substance cannot be derived directly, as neither the PEC, nor the PNEC for the whole substance will be available. The PEC/PNEC ratio is therefore derived from the PEC/PNEC ratios of the "blocks" of components, based on the proportional contribution of each of the "blocks" to the composition of the whole substance, and assuming that effects will be concentration additive:

$$\frac{PEC}{PNEC}\ whole\ substance = \frac{PEC_A}{PNEC_A} + \frac{PEC_B}{PNEC_B} + \frac{PEC_C}{PNEC_C}\ etc. \quad (2)$$

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

This is referred to as the Hydrocarbon Block Method (HBM).

In relation to the above it should be noted that where the petroleum substance is of such limited complexity that it can be considered to constitute a single "block" (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 "block" are the same, the ecotoxicity data used to obtain the PNEC can be based on the toxicity of the whole substance, and the PEC/PNEC ratio can be obtained directly.

Given the complexity of many of the petroleum substances and hence the number of "blocks" that will be created, allied with the need for flexibility in the assessment procedures, it is considered that the use of this method of risk assessment for petroleum substances will, in practice, only be possible using computer based assessment procedures.

In view of the fact that particular "blocks" of hydrocarbons may be present in more then one petroleum substance, there may be a need to consider the contribution to the overall environmental risk from more then one petroleum substance. In principle the HBM allows for calculating the combined environmental risks of different petroleum substances in specific situations or for the comparison of combined PEC values with monitoring data. For this, the PEC/PNECs of the different discharged petroleum substances (or the values for their specific blocks) can be combined in the same way as the blocks for a specific petroleum substance are combined, assuming that the effects will be concentration additive.

3. Outline of the application of the hydrocarbon block method

The following outlines the principal steps in the application of the HBM:

- obtain compositional data for the substance that are sufficient to assign components to "blocks";
- define "blocks" by grouping components on the basis of similar structural and/or physico-chemical properties, degradation parameters and ecotoxicological properties. If desired, "blocks" can be defined as single components;
- obtain production and use data;
- establish release estimates for each "block". A single release estimate for a petroleum substance may not always be adequate: "blocks" with markedly different physico-chemical properties may require different release estimates;
- assign representative values for physico-chemical properties, degradation rate constants and LC/EC50s and NOECs for each "block";
- determine the PEC value for each compartment for each "block" (local as well as regional);
- determine the PNEC value for each "block";
- calculate PEC/PNEC ratio for each "block" and sum proportionally.

Summarising, once the "blocks" with their physico-chemical and ecotoxicological properties are defined, there is no difference between the approach presented in the main text of the Technical Guidance Document and the HBM. This means that a PEC_{local} and $PEC_{regional}$ can be calculated as described in Chapter 2 of the main text and a PNEC can be derived as described in Chapter 3 of the main text.

4. Points for special consideration when using the HBM for risk assessment

The more detailed description of certain aspects of the application of the HBM which follows, is largely based on the application of the HBM to risk assessment for the aquatic environment. This is because it is considered that given the present state of the development of environmental risk assessment, and of the use of the HBM in particular, the use of this compartment best exemplifies the principles, applicability and the issues associated with the use and further development of the HBM.

4.1. Composition of petroleum substances

The composition of many petroleum substances is complex, with a single substance often containing a large number of component chemicals, varying in chemical type, molecular weight and isomeric structure.

For some petroleum substances the differences in the physico-chemical properties of the different "blocks" will be such that a single release estimate for the substance may not be sufficient and separate release estimates for some "blocks" or groups of "blocks" may be required.

The complexity of some petroleum substances is further compounded by the fact that their composition may vary depending on the source of the crude oil from which they are produced and the method of their production. It is therefore necessary, that adequate information be available not only on composition but also, where relevant, on variations in composition. This information can be used to allow several calculations of the PEC/PNEC for a substance to take account of likely variations in composition. For petroleum substances, adequate information on composition may allow risk assessment of groups of substances to be undertaken at the same time, for example whole groups of naphthas or kerosines.

It is clear that for many petroleum substances a complete resolution of the composition is neither achievable nor necessary to be able to carry out a risk assessment. But it is essential that compositional data, including information on variability, is sufficient to allow "blocks" to be properly defined for the purpose of risk assessment.

It should be borne in mind that some petroleum substances will contain a relatively narrow range of components and be much more consistent in composition e.g. some narrow-cut hydrocarbon solvents. In some cases it may be appropriate to regard such substances as a single "block".

Many of the components of petroleum substances will be present in many of the substances. In general it is desirable to ensure, that when similar components are present in different petroleum substances the same approach to "blocking" is taken. This will allow the development of PEC/PNEC ratios for "blocks" applicable to a range of petroleum substances (data on physico-chemical and degradation properties and toxicity values for these "common blocks" will only need to be generated once).

4.2. 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 "block" 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 Kow is the main parameter. This implies that "blocks" can be defined on equally spaced log Kow values: e.g. <3.0; 3-3.5; 3.5-4.0 etc.

It is proposed to start with such a "block definition" for application of the HBM. Based on the results of the risk assessment the "blocks" may be further refined.

4.3. "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.

4.4. Additivity of toxicity

It is generally accepted that for chemicals with the same mode of action, acute toxicities can be considered as additive (EIFAC, 1987). There is increasing evidence that this is also true for chronic toxicity (Hermens, 1989).

Whether a chemical or a group of related chemicals act by non-polar narcosis can be based on a comparison of test results with QSAR estimates for base-line toxicity. Schemes exist that allow the classification of large numbers of organic chemicals according to their mode of action (Verhaar et al., 1992).

Petroleum hydrocarbons are for the great part composed of hydrocarbons. These act via a similar mode of toxic action, non-polar narcosis. In the light of the above it can be assumed that for the hydrocarbon components of petroleum substances, effects will be simple concentration additive.

The situation is less clear with regard to chemicals with different modes of action. Components of petroleum hydrocarbons with specific modes of action are likely to be "blocked" together, provided they have the same specific mode of action. In the first instance the PEC/PNEC ratio of this "block" shall be added to the total PEC/PNEC ratio. From this it will be clear if the PEC/PNEC ratio for that "block" influences any potential for environmental risk for the specific petroleum substance. If it does, further investigation whether or not there is additivity of the modes of action, would be required.

Chemicals which may have a specific mode of action present in petroleum substances can be metallic constituents (e.g. vanadium and nickel in crude oil, fuel oils and asphalt) and heterocyclic compounds (e.g. carbazole compounds in cracked fuels) and mutagens/ carcinogens (e.g. PAHs such as benzo(a)pyrene, 7,12-dimethylbenzo(a)anthracene. However, they are present in low concentrations compared to the non-specific acting components. Nevertheless, these specific acting constituents should on a case-by-case basis be taken into account in the environmental risk assessment at least in a qualitative way.

4.5. QSARs

The identification of the blocks when applying the HBM may be dependent on the use of QSARs for the estimation of physico-chemical properties (e.g. log Kow, water solubility, melting point and vapour pressure) and degradation rates (e.g. photodegradation and hydrolysis rates), when measured values are not available. There are reasonably well accepted methods for the generation of these data using readily available data bases, or QSARs. There are no widely accepted QSARs for biodegradation, but it is considered adequate, at least for screening, if experimentally determined rate constants for the "blocks" of interest are not available, to use QSAR estimates for block identification, according the principles laid down in chapter 4 on the Use of QSARs.

The use of QSARs is well established for predicting the acute toxicity of simple hydrocarbons, and can be used to supplement the available ecotoxicity data. Whilst the accuracy of QSARs for more complex hydrocarbons and for chronic toxicity may need further consideration, they provide an adequate default where experimental data are not available (in particular where the values are found not to be key to the outcome of the risk assessment).

The minimum data-set available for each priority petroleum substances, is usually not sufficient for risk assessment using the HBM, because it will usually comprise tests conducted with the whole petroleum substance. Since in the HBM process individual hydrocarbons are blocked together on the basis of their environmental fate and ecotoxicological properties, additional data on these hydrocarbons are also required. These may be measured data, but it is foreseen that values derived from QSARs will be helpful for filling datagaps in the establishment of blocks. When the overall risk assessment for the petroleum substance is undertaken (with the PEC/PNEC ratios for the blocks calculated and summed), those blocks contributing most to the overall PEC/PNEC ratio can be identified. It should be noted that any decision on the final outcome of the risk assessment when the overall PEC/PNEC ratio is close to or greater than one, will need to be based on measured (rather than QSAR) data. Hence, for each block (unless the contribution of the particular block is found to be irrelevant to the outcome of the risk assessment), representative measured base-set data should be available. These data could be on any component of the block, since by definition, blocks are comprised of hydrocarbons with similar fate and ecotoxicological properties. Data on some individual hydrocarbons suitable for this purpose, are already available as the IUCLID database shows.

For "block" identification, QSARs for short (algae, daphnids and fish) and long term (daphnids and fish) toxicity are given in Chapter 4 on the use of QSARs. These QSARs can be used for chemicals with a non-specific mode of action, i.e. for most petroleum substance components. Considering the assessment factors presented in the TGD (see section 3.3.1 of the main text) a factor of 10 on the QSAR derived long term NOEC is proposed. More guidance on the use of QSARs in general can be found in Chapter 4.

4.6. "Blocks" which do not exhibit acute toxicity

There will be a number of "blocks" for which no acute toxicity is indicated at the limit of water solubility. Adema (1986, 1991) found no short term toxicity for n-decane or higher homologues and for alkylbenzenes with a carbon number higher than 14. This does not necessarily mean that these "blocks" will not contribute to chronic toxic effects. There may be several approaches to estimate chronic toxicity for such chemicals if there are no measured long term toxicity data available:

- use the QSAR for long term toxicity as presented in Chapter 4 of the TGD. However, these QSARs can only be applied in a range of log Kow from approximately 2-6. For chemicals with higher log Kow the resulting NOEC is often higher than the water solubility.
- For blocks which do not demonstrate acute toxicity at or below their water solubility, QSARs (irrespective of the fact that the result may exceed the water solubility) may be used as a basis for the PNEC by application of a suitable assessment factor. This calculated value is taken to represent the PNEC of the block unless, it is itself greater than the water solubility. In this case the water solubility should be substituted as the PNEC. It should be noted that for very high log Kow values, this may lead to unrealistic PNEC values;
- as an indication above log Kow 6, a parabolic equation to derive a BCF for fish can be used (see section 3.8.3.2 of main text and Chapter 4) in combination with the critical body burden concept (McCarty & Mackay, 1982) to calculate the chronic toxicity. This critical body burden concept indicates that the long term critical body burden is equal to the NOEC multiplied by the BCF (CBB = BCF * NOEC) (Sijm et al., 1992, ECETOC, 1995). To be able to perform a risk assessment, there may be a need to develop measured chronic data to support this QSAR prediction.

4.7. 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 $PEC_{regional}$.

4.8. 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.

5. 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.

6. 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.

7. Testing strategies

Based on the identification of the blocks, the estimation of the block properties and the compositional information in combination with exposure scenarios a PEC/PNEC is calculated. If this PEC/PNEC is > 1, the general guidance concerning testing strategy as presented in section 5 of the main text will be followed. Further refinement of the PEC or PNEC may be necessary in order to improve the data estimates for the properties of the blocks.

A form of "sensitivity analysis" may be useful in confirming the selection of blocks to represent a particular petroleum substance; this approach may also be used to identify those particular parameters which are important in defining the fate and effects of the block. This approach may be useful to identify the most relevant additional data that would influence the outcome of the risk assessment.

Further refinement of the data estimates for the block properties should be made when:

- specific blocks have PEC/PNEC values > 1 or;
- the total sum of the blocks results in a PEC/PNEC ratio > 1.

For the blocks with a PEC/PNEC ratio > 1, one or some representative components should be selected. For these component(s) the testing principles from the TGD can be followed and the results can be used as representative for the specific block. If the combination of blocks with individual PEC/PNECs < 1 gives a PEC/PNEC > 1 it is suggested to focus on the major contributing blocks. For the relevant blocks again representative components can be selected and the general testing principles applied.

8. 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.

9. References

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Appendix X: Transformation pathways

In the table below biodegradation and transformation pathways of some organic compounds are summarised. The mechanisms and pathways presented here are not comprehensive and other mechanisms and pathways may therefore occur. It should also be noted that the assessment of transformation pathways may be complicated due to the interaction between different functional groups within a molecule. The following references give further detail:

- Alasdair Neilson, Organic Chemicals in the Aquatic Environment [1994]. Distribution, persistence, and toxicity. ISBN 0-87371-597-7).
- Larson R.A. and Weber E. J. (1994). Reaction Mechanisms in Environmental Organic Chemistry. ISBN 0-87371-258-7.

GROUP	METABOLIC PATHWAY	TRANSFORMATION PRODUCT(S)
Aldehydes	Oxidation	Carboxylic acids
Alkanes, branched	Oxidation/carboxylation	Alcohols/carboxylic acids
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	Carboxylic acids/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

GROUP	METABOLIC PATHWAY	TRANSFORMATION PRODUCT(S)
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	Alkanes, inorg. phosphate
Phenols	Carboxylation (anaerobic)/ oxygenation (aerobic)	Hydroxybenzoates/catechols
Sulfoxides	Reduction	Thioethers, thiols
Sulphonates, aromatic	Elimin. of sulfite by dioxygenation	Catechols
Sulphates, alkyl	Hydrolysis	Alcohols, inorg. sulphate
Ureas	Hydrolysis	Amines

Appendix XI: Environmental risk assessment for ionising substances

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.

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 Kow.

The basic parameters used in the exposure assessment (log Kow, Henry's law constant, adsorption/desorption coefficients) are only applicable to the non-ionised form of the substance. Therefore, every time when partitioning of a substance between water and air or solids is concerned, a correction needs to be made in order to take only the undissociated fraction of the compound into account at a given pH. In practice, this implies that Henry's law constant and Kp in soil, sediment, and suspended solids need to be corrected. This can be done by using the following correction factor:

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

where:

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

The above correction can only be used for partitioning coefficients which refer to the unionised form of the substance. This means that for estimated partitioning coefficients, water solubility and Kow need to be determined for the neutral form. The choice of relevant pH-values to be used in the calculation should be based on the pKa/pKb of the compound in concern and any relevant knowledge of the actual toxic form of the substance. For experimentally determined partition coefficients the need for correction should be assessed on a case by case basis, depending on the pH in the test.

These principles apply also to the fate of the substance in sewage treatment plant. However, since the STP is a well buffered environment, a default pH of 7 can be used in the calculations. The role of pH in the experimental determination of the bioconcentration should also be acknowledged.

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. Risk characterisation

Care should be taken that the PEC and the PNEC in the risk characterisation represent similar conditions. PEC/PNEC comparisons should preferably be made at both sides of the pKa values, within environmentally relevant pH-range. The higher PEC/PNEC ratio should be used in the risk characterisation, following the realistic worst case approach. If it is not possible to carry out a quantitative analysis, the assessor should take the pH effect into account qualitatively.

Appendix XII: Connection to STP in Europe

At the time of the writing of the TGD, the situation in the Member States concerning percentage connection to sewage works is quite diverse. Across the Community, taken as a whole, approximately 70% of the municipal waste water volume is treated at least in primary purification plants (Table 1).

Table 1 *Water Consumption and waste water treatment practices in Europe*

Country	Population	Water[1]	Sewer[2]	No WWT	1° STP	2° STP	All STP[3]	Plants[4]
	millions	l/capita/d	% of pop.	% of pop.	% of pop.	% of pop.	% of pop.	Number
Belgium	10.02	166	80	65	0	35	35	222
Denmark	5.15	257	92	2	0	98	98	1824
W. Germany	61.0	199	92	10	5	85	90	8245
E. Germany	16.70	199	-	38	25	37	62	-
Greece	10.10	-	42	90	1	9	10	12
Spain	38.81	192	80	53	5	42	47	600
France	56.80	225	83	50	15	35	50	8000
Ireland	3.50	-	66	59	17	24	41	540
Italy	57.52	277*	78*	40	15	45	60	3119
Luxembourg	0.39	274	96	17	4	79	83	63
Holland	14.83	213	92	10	2	88	90	475
Portugal	10.40	-	41	65	35	0	35	340
UK	57.60	259	96	17	9	74	83	7750
Austria	7.86	261	75*	28	72		72	500*
Finland	5.00	279	69*	24	76		76	560*
Sweden	8.64	291	86*	5	95		95	1000*
TOTAL	364.32	-	-	33	67		67	-

* 1984

1 Figures for 1991 from 19th International IWSA Congress in October 1993 quoted in; WSA (1994). Waterfacts. Water Service Association: London.

1 Figures for 1988-90 from; Matthews, P.J. (1992). Sewage sludge disposal in the UK: A new challenge for the next twenty years. JIWEM 6(5), 551 – 559.

1 Figures for EU12 from; Morse, G.K., Lester, J.N. & Perry, R. (1994). The economic impact of phosphorus removal from wastewater in the European Union. European Water Pollution Control 4(3), 46-55. Austria, Finland and Sweden from; "Basic Statistics of the Community. Comparison with the principal partners of the Community" (30th ed., 1993) obtained via Eurostat/OECD cooperation and quoted in; European Water Pollution Control 4(2), 35 ("Water Indicators").

1 Figures for 1988-90 from; Matthews, P.J. (1992). Sewage sludge disposal in the UK: A new challenge for the next twenty years. JIWEM 6(5), 551 - 559.

European Commission

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Part II

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