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Environmental Hazard Assessment of Substances

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ENVIRONMENTAL HAZARD ASSESSMENT OF CHEMICALS
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ENVIRONMENTAL HAZARD ASSESSMENT OF CHEMICALS

SUMMARY

The main objective of the work described in this report was the development of a process for the Environmental Hazard Assessment of Substances, including principles and practical approaches. The concept is applicable to all substances, whether "new" or "existing" and to all environmental compartments.

The assessment of whether a substance presents a hazard to organisms in the environment is based on a comparison of the predicted environmental concentration (PEC) with the predicted no effect concentration (PNEC) to organisms in ecosystems.

The extent and nature of the information available to make such a comparison varies for different substances and environments. A practical hazard assessment scheme must allow for this. The process described in this report comprises a universal approach in which the estimation of PEC values is based on exposure model calculations and PNEC values on toxicological data. It should be recognized that where more precise information is available, for example direct observations linking measured concentrations in the environmental compartments of concern with effects, or abscence of effects, on organisms in the corresponding ecosystem, this should take precedence.

The proposed scheme involves a stepwise or sequential process in which increasingly refined estimates of PEC and PNEC can be introduced if necessary and as data become available. Less refined estimates represent more conservative values. Comparison between PEC and PNEC can be made at different stages in the sequence. This makes it possible to reach a conclusion and terminate the assessment at the earliest possible point in the sequence, thus optimising effort and resources. Where PEC exceeds PNEC at an early point in the sequence, it is necessary to proceed further until a later comparison using more refined information proves satisfactory or risk management must be considered. It is not necessary that PEC and PNEC values are at the same level of refinement for PEC:PNEC comparisons.

In the sequential process, PEC values are estimated using predictive mathematical models for two geographical scales: regional and local. For diffuse sources, regional models based on representative environments estimate average environmental concentrations and provide information for the particular substance on environmental compartments of concern (air, water, sediment, soil or biota). Local models are used to estimate concentrations near the point of entry into the environment. The sequence comprises three levels of refinement: a preliminary or "Screening" phase, a "Confirmatory" phase and a final or "Investigative" phase. Different release

patterns are considered (dispersive, diffuse and localised) and the losses of the substance to the environment during the full life cycle (manufacture, formulation, use and disposal) are addressed.

PNEC values can be estimated from toxicological data for the substance concerned. Such data may comprise acute or chronic toxicity measurements for various species in laboratory tests or (less frequently) toxicity measurements made in the field. PNECs may be derived from these data by extrapolation using appropriate "application factors" to allow for differences between the conditions under which the measurements were made and those applying in practice. In the present scheme, these application factors were determined empirically by comparing reliable, validated acute, chronic and field toxicity data for sub-sets from a data base relating to 360 industrial and agricultural chemicals. This comparison indicated that for the majority of the substances listed, to estimate a PNEC from acute toxicity studies (which should involve at least three species from at least two taxa), the lowest of the median effect concentrations (EC_{50}s) should be divided by an application factor of 200. Where chronic toxicity data are available, the PNEC may be derived by dividing the lowest no-observed-effect concentration (NOEC) by 5, whereas the NOEC from a multi-species ecosystem study can be taken directly as the PNEC. Certain categories of substances, for example metals and metal-containing compounds do not appear to fit the general relationships and have been excluded. Other product groups such as petroleum products may also require further consideration.

The Environmental Hazard Assessment follows a pragmatic approach in evaluating PEC/PNEC ratios. Where PNEC exceeds PEC in the evaluation for the regional case, the next step in the assessment is to determine a PEC for the local situation. If PNEC exceeds PEC at the local level, because of the conservative approach it can be concluded that the substance does not constitute an environmental hazard and hence the assessment can be finalised.

Environmental Hazard Assessment of substances is a demanding task. The central challenge is to develop practicable and valid means of reflecting behaviour in highly complex real environments on the basis of inevitably limited test data and models. It is believed that the approach proposed here represents the current state of the art (particularly with respect to application factors and regional models). However, although the basic concepts should be universally applicable, it is not yet possible to work out detailed applications of the scheme for all situations. Environmental Hazard Assessment is evolving rapidly and significant further advances in models or in availability of ecotoxicological data can be expected.

Thus, to date most Environmental Hazard Assessment schemes have concentrated on freshwater systems and much less attention has been paid to sediments, soil or the marine environment. As a reflection of this, for this report it proved possible only to undertake the ecotoxicological evaluation and derivation of PNECs for aquatic organisms.

Furthermore, the concepts presented in the report are at present only worked out for steady-state environmental concentrations resulting from continuous emissions and should not be used for non steady-state situations resulting from intermittent releases such as batch processes.

The proposed approach was evaluated for several representative chemicals with differing properties and for which sufficient data were available. PECs and PNECs were derived from all available data so that for evaluation purposes PEC/PNEC comparisons could be made at as many stages in the sequential process as possible, including greater levels of refinement than needed to indicate absence of hazard according to the step-wise scheme.

This evaluation demonstrated that, for the limited number of substances tested, the proposed approach represents a workable system for the aquatic environment. Based on PEC:PNEC comparisons, further refinement did not alter the final judgement once the criteria for absence of hazard had been satisfied.

For both the exposure estimation and the assessment of effects, further work is required to demonstrate and verify the applicability of the scheme and to develop it further. This would include evaluating the scheme with additional chemicals, extending to other environmental compartments and taking into account non steady-state conditions. The present document should therefore be seen as an initial report.

SECTION 1. INTRODUCTION

The production, distribution, use and disposal of substances lead almost inevitably to their presence in the environment on a localised basis and, in some cases their more widespread occurrence. The way in which substances enter the environment depends on their physico-chemical properties, the production process, including extraction of natural resources and manufacturing, as well as on the pattern of use and the means of disposal.

The environment has a capacity to assimilate substances (to render them harmless by breakdown or dilution) but if this is exceeded damage may ensue. To evaluate the impact on the environment of substances which may be introduced into it, it is necessary to have a hazard assessment process. The hazard posed by a substance is a function of its inherent toxicity to organisms in the environment and the concentration attained.

To develop a process for hazard assessment it is necessary to define the principles, and establish practical approaches for:-

- predicting environmental concentrations (i.e. exposure assessment) and
- estimating maximum safe levels in the environment (i.e. effects assessment).

In the 'Exposure assessment' the concentration a substance will reach in the environment is calculated. The 'Predicted Environmental Concentration' (PEC) can be estimated if it is known how and in what quantity a substance enters the environment and how it is subsequently distributed and transformed. Alternatively, the environmental concentration can be measured.

'Effects assessment' establishes a maximum concentration of a substance not causing adverse effects: the 'Predicted No Effect Concentration' or PNEC. The PNEC is derived from whatever ecotoxicological data are available, using, where appropriate, an application factor to compensate for any restrictions in the data.

There has been considerable recent interest in the development of processes for hazard assessment, focused to an extent by impending changes in legislation at the European Community (EC) level.

The principal purpose of this report is to propose a sound, practical and pragmatic approach for the hazard assessment of substances in the environment, outlining procedures for exposure assessments to obtain PECs and effects assessments to derive PNECs. The schemes developed are mainly based on empirical data and give guidance on the application of the hazard assessment process for most substances. The approach should be considered as the default and can be superseded by improved knowledge, taking into account that it represents "state of the art".

This report is dealing with continuous emissions leading to steady-state environmental concentrations in the relevant compartments. Intermittent releases resulting from batch processes have not yet been covered.

Only hazards related to organisms in the environment are considered in this report. Indirect effects on man (e.g. via taint) will be covered separately. Effects on the physical environment e.g. those causing climate change or ozone depletion are not considered. The report also does not address risk assessment i.e. the probability that a hazard will occur.

In principle, the hazard assessment scheme developed should be applicable to all environmental compartments. Because the aquatic environment is generally regarded as one of the main compartments at risk, emphasis has been placed on the latter in the development and evaluation of the proposed scheme.

It is recognised that hazard assessment is an evolving technique and the method presented here is just one stage in a process which will be subject to refinement. Therefore this is an initial report, in which recommendations to enhance the development of the hazard assessment process are included (Section 7).

SECTION 2. BACKGROUND

2.1 LEGISLATION

On 30th April 1992 the European Council adopted the "7th Amendment" of Directive 67/548/EEC (EEC, 1992a). This will come into force on 30th October 1993. Article 3.2 of this Council Directive requires that risk assessment be carried out according to principles to be laid down in a Commission Directive. This Directive, which requires an evaluation of the potential hazards and risks of notified substances to man as well as the environment, is to be adopted 12 months following the adoption of the 7th Amendment i.e. by 30th April 1993.

The EC proposal for a Council Regulation on the evaluation and control of the environmental risks of existing substances (EEC, 1992b) requires competent authorities to evaluate the real or potential risks of an existing substance to man or the environment. Implementation of the regulation on existing substances is expected by May/June 1993.

Apart from development in the EC legislation, some national authorities have developed similar principles dealing with the evaluation of existing and new chemicals (e.g. UBA, 1990; UBA 1992).

2.2 EXISTING HAZARD ASSESSMENT SCHEMES

The Commission of the European Communities, Directorate General XI, organised a workshop on "Environmental Hazard and Risk Assessment in the Context of Directive 79/831/EEC" (EEC, 1990) in collaboration with the Environmental Institute of the Joint Research Centre Ispra. This workshop discussed and identified common principles for the environmental hazard assessment of substances to achieve a harmonised and transparent procedure for evaluation of new substances within the Community.

At the request of the Commission the conclusions of the 'Ispra workshop' were discussed by various interested organisations. ECETOC (1991) concluded that the outcome of the Ispra workshop formed a good basis for further discussions. The main points of agreement were that the hazard assessment process should be iterative, that exposure scenarios should be developed for 'use-families' (e.g. surfactants and solvents) and that there was a need for differentiation in the assessment process of the exposure from limited point sources (e.g. manufacturing sites) and exposure from diffuse release (e.g. via widespread use of substances).

Several national authorities and international organisations are developing hazard and risk assessment concepts for new and/or existing substances (e.g. Germany, The Netherlands, UK, Switzerland, USA and the OECD).

The Dutch authorities with support from the National Institute of Public Health and Environmental Hygiene (RIVM) have developed hazard and risk assessment schemes (VROM, 1988/89, 1992). Partly as a result of these developments, the Dutch authorities were requested by DG XI to assist with the development of a system for ranking existing substances on the basis of their environmental hazard. They also developed similar schemes for estimating the environmental hazard of new substances and pesticides for the Dutch authorities. The application of an early version of the Dutch hazard/risk assessment scheme for existing substances indicated that a significant number would have restrictions or would have to be abandoned. This may be due to the conservative approach of applying high safety factors, sometimes unsatisfactory input data and stringent default values where data were missing.

At the request of DG XI, the UK authorities have developed a hazard and risk assessment scheme for new substances for incorporation in the '7th Amendment'.

Existing schemes for hazard assessment generally follow a stepwise approach in which, if necessary, increasingly refined estimates of the PEC(s) and PNEC(s) can be compared in a series of stages. Table 1 outlines some existing/proposed environmental hazard assessment schemes together with brief comments on each. Some approaches are restricted to certain categories of substances such as household substances (e.g. AIS, UBA) whereas others are generally applicable to industrial and consumer products/substances. The approaches tend to be conservative in their estimation of environmental concentrations due to a number of assumptions.

TABLE 1 - (Part 1)

COMPARISON OF EXISTING/PROPOSED HAZARD ASSESSMENT SCHEMES

Name	General outline of the procedure	Use pattern	Release estimation	Exposure assessment (Target compartment)	Proposed models for calculation of environmental concentration
CH-Switzerland (Ordinance on substances)[1]	Stepwise procedure: estimation of emissions/ effect data/hazard assessm. /env. risk ass.	- Uses with direct or high emissions - Incorporated into a matrix - Closed systems - Destructive uses	Based on type of use and amount as well as on mode of disposal (see use categories)	Based on assumed distribution into the different env. compartments	No specific models
UBA (Germany)[2]	Definition of degradation and ecotoxicity criteria for ecolabelling of detergents (German "blue angel")	Detergent ingredients (i.e. wide dispersive use) which enter quantitatively sewage and subsequently receiving waters without/after passing sewage treatment	Rough calculation taking into account the total detergent consumption (of the country concerned) and the proportion of each individual ingredient formulation	Calculation of the substance concentration in raw sewage, in sewage plant effluents and receiving waters taking into account substance consumption figures, the proportion of the substance which is eliminated / biodegraded in sewage treatment plants, the per capita sewage output and the dilution factor of the sewage effluent by the receiving water volume.	Emission algorithm. Standard dilution factor (SDF) = 10 is normally used.
VROM (NL)[3]	Stepwise procedure with increasing level of complexity of data (effects and exposure)	Several use categories such as textile dyes, paper chemicals, etc.	Release estimation according to use categories	All environmental compartments: Air, water, soil, sediment.	DRANC; Local models PRISEC: Mackay + local models USES: Mackay + local models
ISPRA (EC)[4]	Stepwise approach (Screening stage, etc.)	Different use categories	- continuous - intermittent - dispersive - non-dispersive	Based on realistic worst case assumptions	No specific models
OECD[5]	Tiered approach: - initial - intermediate - comprehensive	Grouping of substances according to type of use: industrial, public, ... use categories: dye stuff, intermediates, ...	Covering whole life cycle:- - production - processing - use - recycling - disposal and waste treatment	Focused on:- - air - water - soil	3 local models concerned with a single compartment (SAMS) 1 regional/global model (Mackay Level III)

TABLE 1 - (Part 1 cntd.)

COMPARISON OF EXISTING/PROPOSED HAZARD ASSESSMENT SCHEMES

Name	**General outline of the procedure**	**Use pattern**	**Release estimation**	**Exposure assessment (Target compartment)**	**Proposed models for calculation of environmental concentration**
AIS[6]	Stepwise procedure: Screening, confirmatory, investigative phase	Related to detergent substances only	Emission algorithms	Focus on surface water, soil (modification by waste water treatment)	Biodegradation model for screening phase
UK DoE/CIA Model[7]	Iterative: assessment refined as more data on substance becomes available	Point source: direct discharge or via sewage treatment plant. Diffuse: from several sites to whole country	Based on production, use and disposal	Aquatic environment only; removal in STW considered and dilution in river	No specific models

1 BUWAL, 1989
2 UBA, 1991a; 1991b
3 Van de Meent and Toet, 1992
4 EEC, 1990
5 OECD, 1989; 1991
6 AIS, 1989
7 DoE/CIA, 1992

TABLE 1 - (Part 2)

COMPARISON OF EXISTING/PROPOSED HAZARD ASSESSMENT SCHEMES

Name	Proposed (eco-) toxicity tests	PEC / PNEC comparison	Safety factors / Uncertainty factors	Status	General Remarks
CH -Switzerland (Ordinance on substances)	Acute tests (point emissions) Chronic tests (dispersive use)	To be taken into consideration for risk assessment only (2nd stage)	Not explicitly given	Legally required - responsibility of manufacturer / importer	Guidelines provide a useful general instrument for a rough environmental hazard assessment. No strict scheme to be followed. Guidelines give useful specific figures for CH (waste water pro capita, etc.)
UBA	Tolerable effect concentrations are deduced from acute/chronic test data applying assessment factors. Approach is consistent with the ISPRA document.	yes (Ratio of PEC surface water / Tolerable effect concentration)	Depending on the ecotoxicological test data base, assessment factors of 1000 (few acute data), 100 (several acute data) and 10 (chronic data for 3 species) are applied.	Approach forms the basis of the criteria setting for the German ecolabel established for "detergents as a component system". The UBA approach has also been applied for hazard assessment of detergent ingredients by the UBA (cf. DTDMAC discussion).	UBA approach is principally based on the hazard assessment scheme of the ISPRA document. Exposure assessment is expected to yield overestimated PEC values particularly in those cases where the major part of domestic sewage is treated in biological sewage treatment plants.
VROM (NL)	Acute, chronic, more comprehensive tests according to step of the procedure	yes	10 - 1000 (according to test level, using modified EPA approach)	Discussion documents	Env. PEC's are expected to be sometimes overestimated.
ISPRA (EC)	Acute tests Chronic tests Biodegradation tests	yes	Assessment factors 10-times more conservative as comp. to EPA/AIS approach	Summary of a workshop (Oct. 1990)	Confusing description of receiving environment Simple initial env. conc. calculation including corresp. dilution factors.
OECD	Acute/chronic tests; human exposure via food to be considered	yes	10-1000 according to type and number of tests	Effect/hazard assessment: - OECD report no. 26 (1989) Exposure assessment: - Draft report Jan. 1992 (Berlin workshop 1991)	Exposure assessment process in evaluation (different approaches by different member countries) Local models (SAMS) and global model available for testing in May 1992

TABLE 1 - (Part 2) cntd.

COMPARISON OF EXISTING/PROPOSED HAZARD ASSESSMENT SCHEMES

Name	**Proposed (eco-) toxicity tests**	**PEC / PNEC comparison**	**Safety factors / Uncertainty factors**	**Status**	**General Remarks**
AIS	- Acute tests (screening) - Simulation tests (conf. level) - Field trials (invest. stage)	yes	No fixed safety factors. Increasing certainty with increasing level of assessment	Surfactant industry proposal	
UK DoE/CIA Model	Acute and chronic tests	yes PNEC replaced by Env. Conc'n of Concern = Effect Conc'n/Assessment Factor	Assessment factors: 1-1,000 depending on available toxicity data (after US-EPA) Factors may be reduced if data available to suggest this is appropriate.	Official UK proposal to the Commission	A simple approach to the estimation of PEC is adopted and this concentrates primarily on the aqueous phase. Since losses to other environments are ignored probably a "worst case" PEC is obtained

SECTION 3. THE HAZARD ASSESSMENT SCHEME

The hazard assessment scheme proposed in this report is also based on stepwise assessments of predicted environmental concentrations and ecotoxicological no-effect concentration followed by a comparison of these two values. It should be understood that these steps do not have to proceed simultaneously: a PNEC may advance to a highly refined stage even though a PEC is only at the screening level, or vice versa. The scheme is constructed so that whenever the PEC/PNEC is <1.0, it is concluded that the substance does not present an environmental hazard under these conditions. Figure 1 demonstrates the elements of the decision-making process.

The scheme is considered to be applicable, in principle, to all substances irrespective of whether they are 'existing' or 'new', including those which are subject to special regulations (e.g. crop protection products). However, any particular characteristics of the exposure pattern or ecotoxicological effects of families of substances may need to be taken into account and supersede the general approach recommended here. Some of these exceptions will be mentioned in the text.

In general, exposure is defined as a function of both duration and magnitude of the concentration experienced by receiving organisms. However, as already mentioned the hazard assessment scheme proposed is aimed primarily at predicting the hazard of substances expected to be present in the environment on a continuous basis at a relatively constant concentration i.e. in steady-state conditions. It is recognised that in certain situations assessments will need to be made for non-steady-state conditions such as might exist where effluents from batch processes are discharged or where accidental contamination has occurred (Section 4).

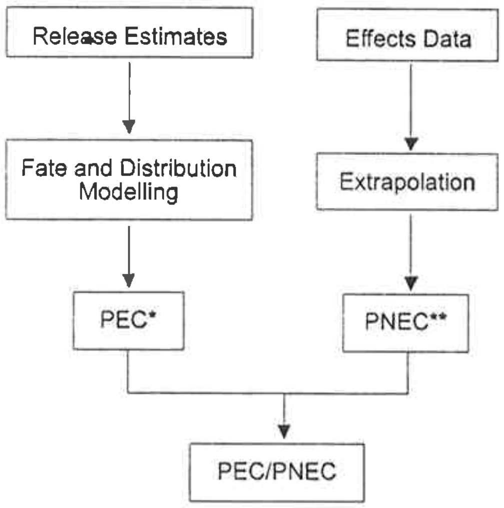
An essential element in the development of such an assessment scheme is the ability to evaluate critically its performance. To examine the performance of the proposed hazard assessment scheme eight substances were chosen, representing a wide range of chemical types and for which an extensive data base on environmental effects and adequate data for environmental exposure assessments were available. The collated data on these substances were used to establish PECs and PNECs within the proposed hazard assessment scheme.

The substances used in the case histories are:

Linear alkylbenzene sulphonate (LAS)
Nitrilotriacetic acid (NTA)
3,4-Dichloroaniline (DCA)
Benzene (BZ)
Diethylhexylphthalate (DEHP)
2,6-Di-tert-butyl-4-methylphenol (BHT)
Cypermethrin (CYP)
Zinc (Zn)

FIGURE 1:

BASIC ELEMENTS OF THE HAZARD ASSESSMENT SCHEME RESULTING IN PEC/PNEC COMPARISONS



* Predicted Environmental Concentration

** Predicted No-Effect Concentration

SECTION 4. EXPOSURE ASSESSMENT

4.1 INTRODUCTION

The objective of exposure assessment is to identify the relevant environmental compartments and to provide information on the resulting steady-state concentrations. These concentrations can be measured directly or predicted by using appropriate mathematical models.

Substances emitted during their production, use and disposal will enter the environment directly or via treatment facilities. After distribution, they may be present in one or more environmental compartments, such as air, water, soil, sediment or biota.

Substances can be released into the environment from single or multiple point sources or from diffuse sources. The type of source will strongly influence the release estimation and will determine the type of mathematical model to be used for predicting the fate and distribution of the substance. This will be shown in the following sections.

Because the environment consists of many interacting elements subjected to temporal and spatial variations which are also not fully understood, every model approach to predict environmental concentrations is a simplification of the real situation. Consequently, substances have to be assessed in so called generic or evaluative environments, which have standardised but realistic properties such as composition, temperature, volume and so on. Before a model can be used with confidence to predict environmental concentrations, it needs to be validated.

Exposure assessment will be applied to new as well as to existing substances. For new substances this assessment is the basis for the evaluation whether there might be a potential environmental hazard connected with the planned volume of production, use and disposal of the substance. Thus, it is essential for competent authorities and industry to have a common and broadly accepted process for estimating environmental concentrations under realistic conditions. With regard to existing substances, only a limited number of well documented measurements are available for specific substances. But even these data cannot cover the whole variability of the environmental conditions so that again recourse to models is necessary.

4.2 GENERAL PROCESS

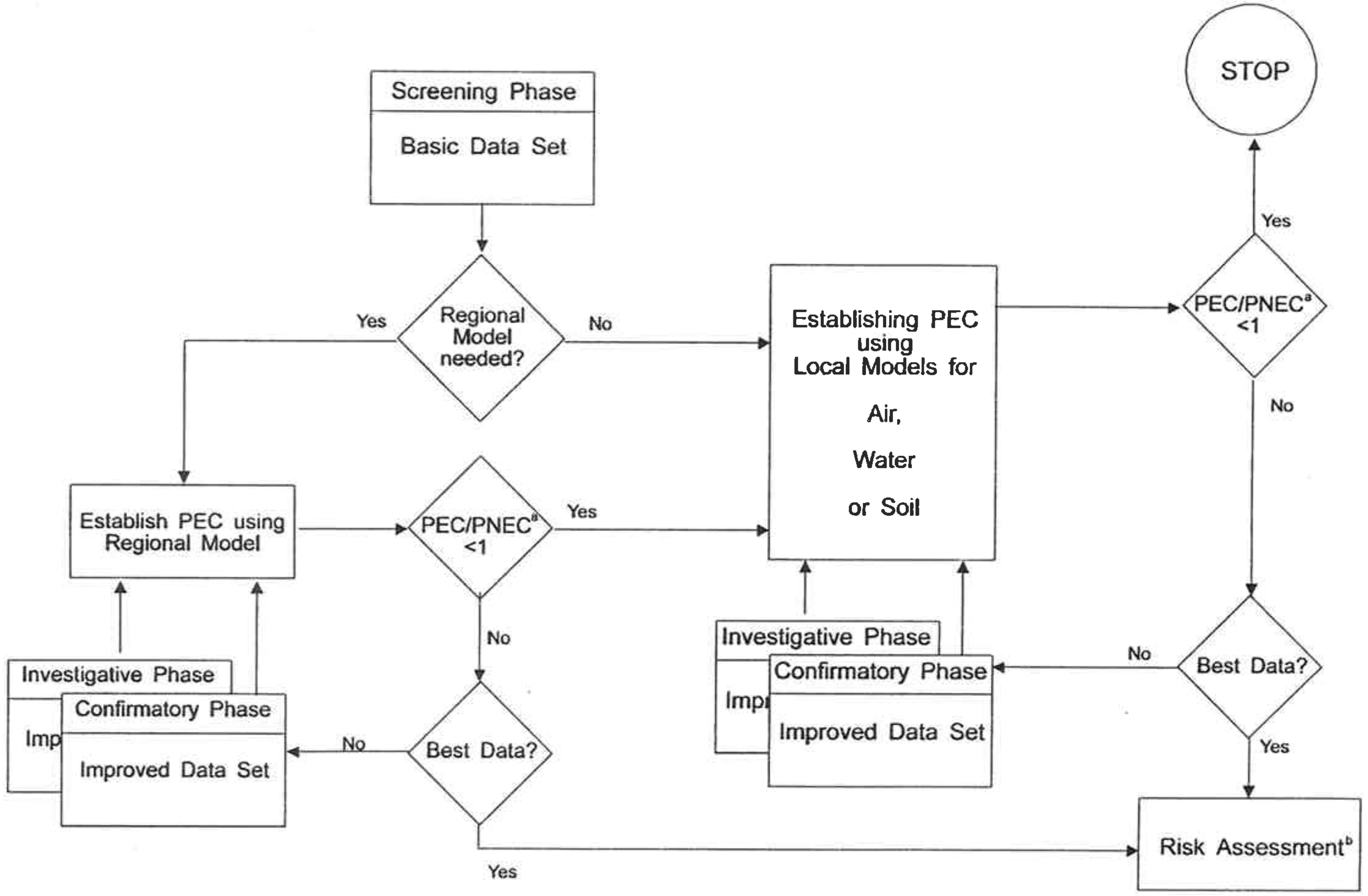
In common with most other schemes, a stepwise or iterative approach is proposed in which the principal decision points involve a comparison of the predicted environmental concentration with the predicted no-effect concentration. The basic scheme is outlined in Fig. 2. The following notes have been included to explain the philosophy, assumptions and general principles on which the scheme is based.

Three phases, called Screening, Confirmatory and Investigative are related to the level of detail of the data used. The nature and quality of the data needed in the separate phases is described in detail in Table 3 (Section 4.3.2). The process involves the use of regional and local mathematical models. The decision to run a regional model will depend upon the use and release pattern of the substance. Non-dispersively used substances and substances used in a closed system or enclosed in a matrix, may not need an evaluation in a regional model if emissions arise only from a limited number of single point sources.

In the subsequent steps in the assessment, more realistic and reliable predictive data are generated and the uncertainties associated with the estimations of PECs diminish. In the screening phase, conservative generic assumptions for the release factor and the dilution/elimination factors are used, whereas in the confirmatory phase, the assumptions concerning the release factors and the dilution/elimination factors will be refined with more detailed information about use pattern, elimination, dilution and transformation in the receiving compartments. The use of additional uncertainty factors for the PEC estimation is therefore not necessary.

Before proceeding to a detailed explanation of the exposure scheme, some general observations regarding the regional and local models are necessary. Generic environmental scenarios will need to be standardized and accepted by both regulators and industry. Environmental parameters such as dilution in rivers, air or soil should be agreed on a scientific basis. The regional model calculates essentially steady-state concentrations in the various environmental compartments using a specific volume for each compartment in a generic region. The homogenous partitioning of the substance among completely mixed compartment volumes is not attained in reality and hence the values obtained for the PECs represent average values, which are often exceeded locally (function of release pattern and use). The local air, water or soil models are therefore designed to complement the regional model and to refine the prediction of actual substance concentrations for the compartment of concern/interest near or at the source of emission.

FIGURE 2
PROCESS SCHEME EXPOSURE ASSESSMENT
(Establishment and Refinement of PEC)



a Use PNEC from Figure 4

b Only if best data for PEC and PNEC were used.

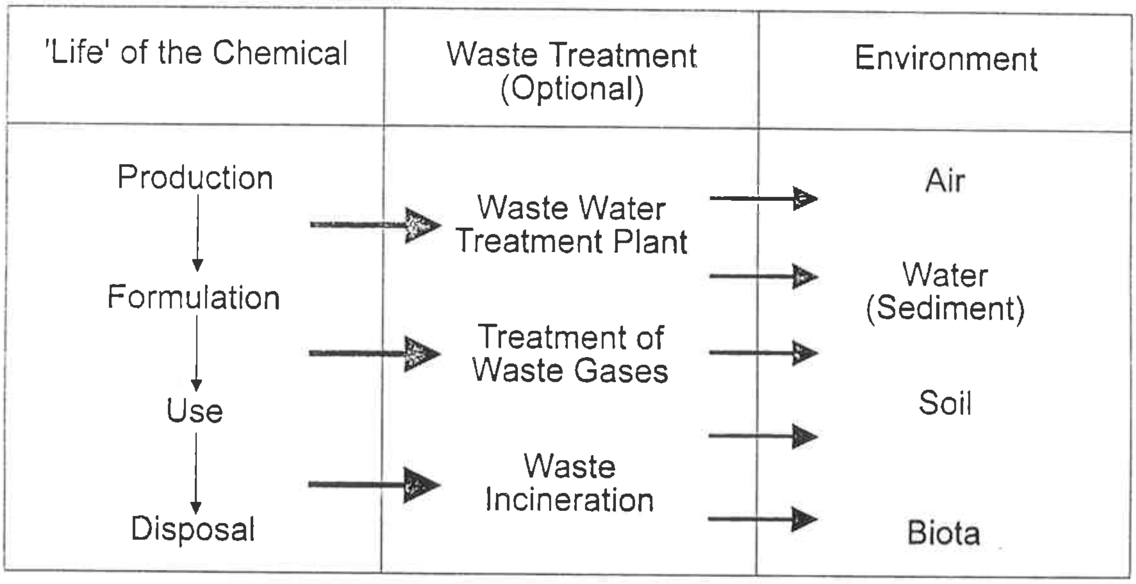
For substances showing a PEC/PNEC ratio > 1, a subsequent step in the hazard assessment is necessary. More refined information on, for example, photodegradation in air may radically modify the outcome. To obtain more detailed data on critical parameters, further application of models might be considered worthwhile steps in such cases.

4.2.1 RELEASE ESTIMATION

Estimation of the release of a substance to air, water and soil is the first step in exposure assessment. It involves an initial estimate of the amounts of material released into the different environmental compartments and provides the basic input for environmental modelling. Therefore realistic release estimates are crucial for calculating environmental concentrations.

As indicated in Figure 3, emissions into the environment may occur throughout the 'life' of a substance, starting with production through formulation and use until ultimate disposal or destruction.

FIGURE 3
EMISSIONS OF A SUBSTANCE INTO THE ENVIRONMENT
(without recycling)



When estimating releases it is necessary to assess whether the amount of material produced and waste generated will be modified by recycling steps and whether, prior to discharge into the environment, effluents will be treated in a waste water treatment plant, an air scrubber or a solid waste incineration facility.

The emission pattern, the quantities released into the different environmental compartments and the number of emission points during the 'life' of a substance varies widely depending on how it is manufactured, formulated, used and finally disposed of. For instance in the case of intermediates used for chemical production only a very small fraction of the amount produced will usually be released into the environment, whereas in the case of products used in the household e.g. detergents, almost 100% will be discharged into the public sewer.

Emissions may arise from **point sources** - either single or multiple - or from **diffuse release**. A typical example of a point source would be a chemical intermediate used at one production site, while solvents would represent a classic example for diffuse release. However, a large number of point sources with frequent emissions may also result in a diffuse release pattern (e.g. automobile exhaust gases, household detergents). Furthermore, emissions can be continuous (e.g. solvents, detergents), intermittent or seasonal (e.g. plant protection products).

To standardize and simplify the release estimation the EEC/OECD have defined different categories of use pattern with regard to the proposed Regulation on Existing Substances. These categories are 'Main', 'Industrial' and 'Use' and reflect a different degree of resolution.

The 'Main' category classifies the substances in four groups (Table 2). In addition, there are 15 different 'Industrial categories' and 55 different 'Use categories' defined (Hedset, 1992). This means that all existing substances have to be classified accordingly by assigning at least one element of each category to it.

Example:	LAS (Linear Alkylbenzenesulfonate)	
	'Main' wide dispersive use	
	'Industrial'	personal and domestic use
	'Use'	cleaning/washing agents and disinfectants

This classification scheme allows a tiered approach in release estimation. This means that in the screening phase a rough estimate based on 'Main' category may be sufficient, whereas in the confirmatory phase more refined release data e.g. based on 'Industrial/Use' categories are needed. In the investigative phase, detailed information on the specific releases of the substance is necessary.

Based on the different categories, emission scenarios are prepared by the authorities as well as by industry. The first proposals for defining release scenarios were presented at

TABLE 2
RELEASE FRACTIONS IN THE SCREENING PHASE RELATED TO THE MAIN CATEGORIES

Main category	Release fraction of production volume	Examples
Closed system	0.01	Chemical Intermediate
Enclosed in a matrix	0.1	Plastic additives
Non dispersive	0.2	Photochemicals
Wide dispersive use	1.0	Solvents, plant protection products, detergents

the Ispra Workshop in 1990. For some groups of substances, e.g. paper chemicals, photographic chemicals and textile dyes, national authorities have sponsored studies to define the emissions associated with the use of these substances (Ros, 1985; Ros and Berns, 1988; Baumann *et al*, 1988). Further work should concentrate on developing such release scenarios to cover a complete range of use patterns. In order to avoid unrealistic exposure estimates, these release scenarios should be validated by comparison with measured data. There is also a difference between release estimation on a regional and local basis. For the estimation of background levels of a substance on a **regional basis** only the overall emissions of a substance into the different environmental compartments are assessed, while the nature, the frequency and the duration of the emissions and the prevailing local conditions are not considered. The following standard emission fractions depending on the 'Main' category of a substance have been proposed (IPS, 1992) as inputs for the **screening phase** (Table 2).

In the **confirmatory phase** generic release data for the corresponding 'Use' category could be used. In the case of chemical intermediates it may be appropriate to divide the 'closed system' group into subgroups with release fractions based on production volume ranging from 0.0001 in the case of products only handled internally in strictly closed systems up to 0.01 in the case of intermediates produced or processed in a large number of sites (Appendix A).

In **the investigative phase** an expert judgement on the particular compound under consideration will be needed. Also, the model for the waste water treatment plant should be refined from a generic to a more specific one.

Local emissions are often discontinuous, especially when substances are processed in batches. Therefore frequency and duration of the emission and local conditions have to be considered. Usually the use pattern will already give some indications as to the main emission points and the relevant environmental compartments (e.g. emissions for a chemical intermediate will occur mainly during production and processing into air and water, for a dyestuff during processing (use) into water, for household detergents after use into the sewer, for a solvent during use into air). For the confirmatory phase generic release scenarios should be developed to cover typical use patterns, including specific use parameters (e.g. typical fixing rates for dyestuffs, volatilisation of polymer additives into ambient air during formulation/extrusion etc.). In addition realistic worse case scenarios are needed for the sites where the substances are used.

Emission to waste water treatment facility.

When emission of a substance occurs via a waste water treatment plant (WWTP), such as for many household and industrial substances, waste water treatment models can be used to estimate concentrations in the aquatic effluents, the gaseous emissions and in the sewage sludge produced.

Screening Phase. In the screening phase, for exposure assessment in water, a simple elimination factor calculated from ready biodegradability data, the Henry coefficient and the log Pow may be sufficient. As shown in Appendix B for industrial waste water treatment plants, the elimination factors proposed at the Ispra workshop significantly underestimate the observed elimination.

Instead of simple elimination factors, mathematical models for WWTP can be used in the screening phase (e.g. WWTREAT and SIMPLETREAT). The major difference between these models is, that WWTREAT (Cowan *et al*, 1992) assumes the total substance and not just the dissolved substance to be available for biodegradation. The sorption to sludge solids increases the residence time of the substance in the WWTP thus potentially increasing biodegradation.

Models can be used to estimate the total percentage of removal such as the percentage of biodegradation of the substance. Performance of these and other sewage treatment models is currently subject of discussion.

Confirmatory/Investigative Phases. In the confirmatory and the investigative phase, models with more specific parameters should be used, which may include results of simulation tests or measured typical concentrations of the substance in waste water entering and leaving the waste water treatment plant as well as measured concentrations in waste air and solid waste.

4.2.2. FATE AND BEHAVIOUR

When released into the environment, substances will be subject to transport and transformation processes. These processes, together with emission patterns, environmental parameters and physico-chemical properties of the substances, will govern their distribution between and concentration within environmental compartments, such as water, air, soil, sediment and biomass. This subject was discussed in detail in ECETOC Technical Report No. 50 (ECETOC, 1992).

Transport may occur within and between environmental compartments. Within compartments advection and dispersion are the dominant processes. By advection substances move along with the flow of the environmental media away from the point of entry and due to turbulence within the media they are dispersed, i.e. diluted.

Rates of advection and dispersion are determined solely by environmental parameters, such as current speed and temperature of the media. In air, rates are usually very fast while in water they may vary widely from very rapid in fast-flowing rivers to very slow in stagnant lakes or ponds. In soil and sediment these rates may be insignificant.

Between compartments, substances can be transferred via processes such as volatilisation, adsorption, wet deposition and sedimentation.

Important transformation processes are biodegradation, hydrolysis and phototransformation. The mechanism of these processes and their rates may vary greatly between and within environmental phases dependent on the reactivity of the substance and environmental parameters, such as temperature, number of active bacteria and solar light intensity.

4.2.3 ENVIRONMENTAL CONCENTRATIONS

General.

The diversity and variability of the environment and of emission sources is often such that substance concentrations in the environment show large temporal and spatial variation.

This is also clear from a compilation of monitoring data for 68 different organic substances in different environmental compartments (ECETOC, 1988). With the exception of sampling points at emission sources it was found that, for these substances, environmental concentrations do not exceed 15 µg/kg in air and 30 µg/kg in water.

It should be noted that monitoring usually is done only at places where chemicals are expected to be present in measurable quantities and that negative findings are rarely reported. Therefore, monitoring data are likely to represent predominantly the higher end of the range of concentrations that may occur in the environment while information on the extent of the area where these concentrations are found is often lacking.

Air.

When transport processes are fast and no boundaries exist as in air, substances can be dissipated rapidly over large areas. Also transformation in air is often very rapid, the most important process being reaction with hydroxyl radicals, but other photochemically formed reactive species, such as ozone, and direct photolysis may also play a role. Reaction - half-lives of only a few days or less are not uncommon (Atkinson, 1986). Because of these rapid rates of transport and transformation, more or less constant and often very low average or background concentrations may be found distant from sources.

Water.

In surface waters, advective transport may be rapid but dispersion and thus dilution is limited by the volume of the receiving aquatic system. Transfer to other environmental compartments, such as sediment and air, is for many substances an important process of removal from water. The rate of transformation processes, predominantly biodegradation and hydrolysis, may be rapid, reaction half-lives being a few days, but for many substances it is much longer. As a result of these processes concentrations of substances dissolved in water usually decrease gradually with distance from sources.

Soil.

In top soil, advection and dispersion are relatively slow. Transformation processes, such as biodegradation, hydrolysis and oxidation, are usually more important for reduction of concentrations. Therefore, in most cases sharp concentration gradients are observed in the vicinity of sources.

Sediment.

Similarly, in sediment advection and dispersion are slow in most cases while transformation may be more important. However, because the substances are supplied via the water phase this may cause a wider distribution, and flatter concentration gradients can be observed in sediment when compared to soil.

Biomass.

For biomass, two different modes of transport or uptake in organisms can be distinguished. Passive uptake occurs via skin and/or gills while active uptake, food chain uptake, occurs via the digestive tract. Passive uptake can be quantified as a function of the substance concentration in the relevant environmental compartment, substance partition coefficients and the rate of excretion from and transformation or metabolism in an organism. The bioconcentration factor is the ratio of the concentration in the biomass and the concentration in the relevant environmental compartments. Biomagnification is the bioaccumulation which occurs through uptake, mainly via the food chain.

For aquatic organisms, the principal mechanism of uptake is passive uptake via the skin and gills of truly dissolved substances, whereas for organisms living in soil and sediment, both mechanisms are involved. Thus, the concentrations in sediment and soil are also important. For plants, uptake may occur through passive uptake from water (aquatic plants) or air (terrestrial plants) via the leaves but also through passive or active uptake from (pore) water via the roots.

Uptake and subsequent concentrations in biomass depend on the bioavailability of the substances. As an example, observed substance concentrations in surface water often include the fraction of the substances that is associated with suspended solids which are difficult to remove. However, for passive uptake in biomass only the truly dissolved substances will play a role, the concentration of which may be substantially lower. Monitoring data often are related to the total concentration of the substance in a compartment. Thus, estimation based on monitoring data can lead to an overestimation of the concentration in the organism.

4.3 MODELS FOR ESTIMATION OF ENVIRONMENTAL CONCENTRATIONS

The effect of transport and transformation processes on the distribution and concentration of substances in the environment may be assessed by using mathematical models (OECD, 1989; OECD,1991; Braat *et al*, 1991; ECETOC, 1992) or studied in experimental models, such as microcosm or mesocosm systems.

As indicated previously, large temporal and spatial differences in substance concentrations may be observed in the environment. The extent of the area and the duration of concentrations in excess of given criteria is often difficult to assess.

As a first step, simple calculations can be used to provide a rough but realistic estimate of substance concentrations in the vicinity of sources. If required, in a second stage more refined and dedicated mathematical models can be applied that include a statistical evaluation of the potential variability of environmental concentrations. In these latter models transformation processes should also be taken into account. Only in cases where the PEC/PNEC ratio is >1, field studies may be performed which can include monitoring at selected sites. These studies would not require mathematical models and will therefore not be considered further in the next section.

The data requirements for mathematical model calculations and the application of different types of models will be discussed in the following sections.

4.3.1 SCOPE AND LIMITATIONS OF EXISTING MODELS

Compilations of existing environmental exposure models have been published (OECD, 1989; OECD,1991; Braat *et al*, 1991; ECETOC, 1992) and the scope and limitations of selected models have been discussed (ECETOC, 1992).

Depending on emission characteristics and the scope of the study, different types of models may be used. The emission characteristics or the discharge pattern of substances into the environment may vary from local to dispersive, well defined to diffuse, single to numerous, stationary to non-stationary, large to small, continuous to discontinuous. Based on these characteristics a distinction can be made between regional and local sources.

Regional Sources.

Regional sources may be dispersive or diffuse. Diffuse sources are often small, not stationary and widely distributed, such as traffic. It may not be possible to identify and evaluate concentration profiles for each single source. In combination, these sources may affect large regions. Dispersive sources are also numerous and widely distributed but they are stationary and can be sufficiently well defined so that each source can be identified and described. However, because of the number and distribution, when combined, they also may affect large regions.

Local Sources.

Local sources can be a single source or several sources which are spaced more or less widely. If there are several sources, concentration profiles may overlap so that the contributions of the different sources have to be summed.

Regional Models.

In the screening phase, simple multi-media models can be used which take into account partitioning between and transformation within the various environmental compartments under steady-state conditions. Currently used and potentially suitable models are HAZCHEM (ten Berge, 1992) which has been derived from a Mackay type level 3 model (Mackay and Paterson, 1991; ECETOC, 1992), and PRISEC, Dutch PRiority Setting system for Existing Chemicals (van de Meent and Toet, 1992).

As already mentioned, these models use generic or evaluative environments which have standardised but realistic properties and represent average situations.

In multi-media models several environmental phases or compartments, such as water, air, soil, sediment and biomass, are represented by separate boxes and complete mixing in each box is assumed. The models calculate average concentrations in each of these environmental compartments which may represent very large areas or volumes. However, as complete mixing seldom occurs in reality, it is likely that there are large areas in a region where concentrations are below background, while they may be higher by several orders of magnitude in much smaller, but still substantial areas.

It is considered that the Mackay Level 3 Fugacity Model is the most appropriate for screening purposes, because it takes into account almost all processes involved in the distribution and fate of a substance:

- partitioning between the air, water and solid phases within compartments,
- degradation and advection in compartments,
- non-equilibrium between compartments,
- mass transfer between compartments driven by non-equilibrium between compartments.

As discussed above, calculated PECs will vary according to the generic environmental scenario and may therefore underestimate actual values (exception should be noted for substances released dispersively or with diffuse uses). Nevertheless, the regional model performs a number of useful functions and provides essential information which is required before progressing to the local model. Although it seems unlikely that many substances will indicate a concern at this stage, the application of the regional model provides appropriate information required for the next stage.

The regional model approach can be used to:

- identify environmental compartments of concern
- provide information on average levels
- identify sensitive parameters
- identify data gaps
- allow substances to be ranked on basis of PEC/PNEC ratios
- set priorities.

Local Models.

The level of detail and sophistication of the air, water or soil model formulation will vary depending on the intended aim. Local models can be used to estimate (maximum) exposure levels in target compartments (screening phase) and/or to quantify temporal and spatial variations in concentrations at some distance from emission sources (confirmatory and investigative phase).

Screening Phase.

In the screening phase, simple calculations can be done which in principle consist of a release estimation (including waste treatment facility) and an appropriate dilution factor.

> **Emissions to Surface Water.** For consumer products, the emission algorithms are often simple. It can be assumed that more than 99% of the release occurs during use. Estimation of the likely concentrations of the consumer products in raw sewage is relatively simple and reliable, given information on quantities of the substances used (per capita and day) and data on the per capita flows of waste water (e.g. 200l per capita and day). For surface water, single stream dilution factors can be used, that have to be agreed between governmental authorities and industry. (For example, for household detergents a dilution factor of 10 is agreed between governmental authorities and the industry).
>
> For other groups of substances, e.g. dyestuffs, more detailed information about use is necessary. Examples for calculations are given in Section 6.1.2.

Emissions to Air. For air, simple screening is performed using the so-called R 91 Report (ECETOC, 1992, Compendium A) or the more refined model VDI 3738 (ECETOC 1992, Compendium B).

Emissions to Soil. For appropriate cases, sludge application factors can be used assuming complete mixing of maximum allowed amounts of sludge within the top layer of the soil. For pesticides, for example, application factors can be used that assume complete mixing of the amount of pesticide applied within the top 5 cm layer of the soil (FAO, 1989).

Confirmatory/Investigative Phases.

In the confirmatory phase, the release estimations have to be refined and site-specific. Dedicated models or suitable simulation tests should be used that can be adapted to the local situation and are suited for the specific problem and compartment of concern. For multiple sources, such models should include a statistical evaluation to account for the variability of local, site specific environmental parameters, such as wind speed and direction of current speed, and differences in discharge characteristics.

Simulation of the dynamic fate and transformation rates of the substance in representative test systems could allow further refinement of the chemical input data. The degradation rates and physico-chemical parameters will be further refined by experimental measurements.

In the investigative phase, the model results need to be validated by comparison to laboratory and monitoring data, taking into account the variability of the concentrations with time related to steady-state and non steady-state situations.

Emission to Water. For surface water, various models are developed. For rivers, SAMS which has been prepared for the OECD (Matthies *et al*, 1992), PDM3 (ECETOC, 1992, Compendium H) and PGROUT (ECETOC, 1992, Compendium I) can be used. Also the model DILMOD is available, having been developed for typical Dutch surface waters. For rivers, ponds and lakes the models EXAMS (ECETOC, 1992, Compendium J) and WASP4 (ECETOC, 1992, Compendium K) can be applied, where the latter model is also suited for estuaries.

Emission to Air. The models TA-Luft (ECETOC, 1992, Compendium D) and PLUIM PLUS (TNO, 1989) provide frequency distributions of air-borne concentrations at ground level. For specific situations many other models are available (ECETOC, 1992). The model SAMS (Matthies *et al*, 1992) calculates air concentrations resulting from different types of sources, area and point sources.

Emission to Soil. For soil, predominantly pesticide application models like PRZM (ECETOC, 1992, Compendium N) have been developed to describe fate and behaviour of pesticides in the root zone and their potential to leach into groundwater for typical soil in the USA. PELMO is derived from PRZM but adapted for typical soils in Germany. Obviously, these models can be used also for non-pesticide substances. The model SAMS (Matthies *et al*, 1992) includes also a module for soil allowing modification of all input parameters required for the calculations.

4.3.2. DATA REQUIREMENTS

There is no restriction on the quality of the initial data used but this of course will determine the level of uncertainty in results and classify the process as screening, confirmatory or investigative. A guide to the quality of the data required for each phase is given below. Clearly, for some existing substances were the necessary data are already available, it will be possible to progress directly to the investigative phase. Conversely, for new materials, the initial studies will involve only the base set data. Again, as indicated for the regional model, the process can be used iteratively with additional and improved data being obtained at each step.

Regional model.

The general condition for using a regional model for exposure estimation should be a dispersive use pattern as observed for consumer products or industrial substances with a wide application area. Generic environmental scenarios will need to be standardized and accepted by both regulators and industry at the screening phase. Environmental parameters such as water/land ratios, compartmental volumes, and residence times should be agreed, as far as is possible, on a scientific basis. This will determine the dilution and available time for the substance to degrade, and therefore determine the reliability of predicted environmental concentrations. Together with exposure estimation, the regional model (Mackay multimedia model level 3) is used for the indication of the compartments where the substance ends up.

TABLE 3
NATURE AND QUALITY OF DATA NEEDED IN DIFFERENT PHASES

Phase	**Quality of Input Data**	
	Release Data	Fate & Phys. Chem. Data
Screening	Initial approximation of anticipated production, emission, uses and disposal.	Base set data (see 7th Amendment). Extent of primary biodegradation estimated from ready test data.
Confirmatory	Detailed data on likely production volumes, reliable estimates on emissions, use and disposal.	Primary biodegradation obtained from laboratory simulation test data, analytical methods, e.g. for degradation products, etc.
Investigative	Accurate knowledge of production corrected for imports and exports, 'measured' emissions, full data on use patterns and disposal.	Field studies, monitoring data.

In the regional model the following groups of data are required:

- Production, use and disposal pattern of the substance
- Physico-chemical data of the substance
- Data on reactivity or stability of the substance
- Characteristics of the mostly used waste water treatment plant
- Characteristics of the regional environment
- Mass transfer factors (kinetic parameters) describing the exchange processes between the environmental compartments

Details are explained in Appendix C. A sensitivity analysis of these parameters is recommended.

Local model.

Examples for data requirements for local environmental fate models are given in ECETOC Technical Report No. 50 (ECETOC, 1992).

SECTION 5. EFFECTS ASSESSMENT

5.1 INTRODUCTION

This section describes the process by which a Predicted No Effect Concentration (PNEC) may be derived from laboratory, field or theoretical data on a substance.

The information available from which a PNEC has to be derived may be of variable size and quality. The process outlined here takes account of this potentially diverse input.

For a large number of substances the data available are very limited.To maximise the effective use of existing data on a substance and to efficiently identify any requirement for new data, it is necessary to have, in outline, a process in which the data will be utilised to determine the PNEC and a description of how the PNEC will be used to make the hazard assessment. A linked series of Process Maps has therefore been constructed which, given a knowledge of the effects data available for a substance, can be used in conjunction with PECs to determine if additional data are required to allow a confident prediction of whether or not there is likely to be an unacceptable hazard to the environment.

Data on a given substance are rarely sufficient to indicate the PNEC without the application of a factor to compensate for uncertainties in the predictive power of the data or to provide an extra measure of safety. In this document these factors are termed "Application Factors" (AF).

The size of an application factor depends on two aspects of the data:

- Ecological relevance: Data from short-term studies in the laboratory generally need large AFs; data from long-term laboratory studies or ecosystem field studies need smaller AFs.
- Number of studies: The minimum data set at the acute or chronic level should be three studies on at least two taxonomic groups; at the ecosystem level one carefully conducted study on appropriate species or communities should be sufficient.

5.2 DERIVATION OF APPLICATION FACTORS FOR LONG-TERM STEADY-STATE EXPOSURE

The PNEC is estimated from acute or chronic data originating in laboratory or field (ecosystem) studies. The three Application Factors necessary for this estimation are :

AF1 - derives the PNEC from acute laboratory studies.
AF2 - derives the PNEC from chronic laboratory studies.
AF3 - derives the PNEC from ecosystem studies.

In reality, AF1-3 are built up from smaller elements:

F1 - Acute:chronic ratio (5.2.1, below)
F2 - Chronic:ecosystem ratio (5.2.2)
F3 - Ecosystem:PNEC ratio (5.2.3)

These three ratios are multiplied together to give AF1-3. Thus:

AF1 = F1 x F2 x F3
AF2 = F2 x F3
AF3 = F3

In addition the need to incorporate factors which describe the relative susceptibility of the recommended "standard species" (as given in EC and OECD guidelines) compared with other species was investigated but found not to be needed: any particular sensitivity of the standard species constitutes an extra, unstated, safety factor.

To provide a scientific basis for the choice of F1, F2 and F3, use was made of an ecotoxicological data base (Aquatic Hazard Assessment database - AHA), extracted from the published literature according to strict selection criteria (ECETOC, in prep.). The database currently contains information on 360 substances tested against 120 marine and freshwater species. Systems for the retrieval and analysis of data were developed and used to derive the Application Factors F1 - F3 (Appendix D).

AFs were initially derived for all substances in the AHA database and subsequently for subsets, excluding inorganics, organo-metals and active ingredients of agrochemicals. Although there were sufficient data in the AHA database to derive F1 and F2, there were relatively few data for the calculation of F3. The AHA database was therefore supplemented with information on ecosystem studies for ten active ingredients of agricultural substances (Appendix D).

5.2.1 ACUTE:CHRONIC RATIOS (F1)

Acute:Chronic (A:C) ratios were derived from the AHA database as follows and with the rules for procedure set out below:

- The acute values were $L(E)C_{50}$s.
- The chronic values were NOECs.
- Any substance having only one $L(E)C_{50}$ and one NOEC was rejected.
- All inorganic substances and organo-metals were excluded (Appendix D).

The geometric means of the acute $L(E)C_{50}$ and chronic NOEC for each substance were established. The ratio between these means was then calculated and the substances ranked by their ratios. The ratios obtained were then plotted as accumulative percentage so that the median and 90 percentile values could be obtained (Appendix D), i.e. the A:C ratio which was greater than or equal to the ratio for 90 % of the substances in the analysis was reported.

The number of substances available for each analysis chosen ranged from 5 to 58. The 90%-ile A:C ratios for substances other than active ingredients of agricultural chemicals fell in the range 27 to 40. Median A:C ratios for all substances fell in the range 4.2 to 22.

Conclusion. Given that the factors are based on 90 percent of substances in each analysis, and that a conservative approach should be adopted at this stage, it is appropriate to set the F1 derived from the A:C ratio at 40.

5.2.2 CHRONIC:ECOSYSTEM RATIOS (F2)

The AHA database contained three substances for which an ecosystem NOEC could be compared with a NOEC from chronic laboratory studies. These data were therefore supplemented with information on ten active ingredients of agricultural chemicals (Pflüger, 1992). The justification for using the data for the active ingredients is that it is considered that these substances have been the subject of some of the best ecotoxicological studies and therefore that they represent the best possibility at present of investigating the Chronic:Ecosystem NOECs ratio. To generate the Chronic:Ecosystem ratios, the lowest NOEC values available were taken for each substance. Where several were available for the same species and endpoint the geometric mean was calculated. The full data are given in Appendix D.

For the ten active ingredients the ratio was 1.6 or less, and for 6 of them the ratio was less than one, i.e. the result from laboratory studies suggested a greater susceptibility to the active ingredients than was observed in ecosystem studies. For the other substances the ratios ranged from 1.3 to 6.3. The 90 percentile for all 13 was 5.2, and included all but one substance.

Conclusion. It is proposed that the factor used to predict an ecosystem NOEC from a chronic laboratory NOEC (F2) should be 5.0.

5.2.3 RATIO OF ECOSYSTEM NOEC:TRUE FIELD NO EFFECT CONCENTRATION (F3)

Given that the true No Effect Concentration cannot be determined, it is considered that a NOEC from a well-conducted ecosystem study will not require an application factor, i.e. F3=1.0.

5.2.4 DERIVED APPLICATION FACTORS

From the above it can be seen that

AF1 = 40x5x1 = 200
AF2 = 5x1 = 5
AF3 = 1 = 1

Thus a PNEC from a satisfactory set of acute toxicity data is 0,005 of the lowest EC_{50}; PNEC from a set of chronic data is 0.2 of the lowest NOEC and from a well-conducted ecosystem study it is the NOEC of that study.

5.3 PROCESS MAPS

The Process Maps summarized in Figure 4 and detailed in Appendix F indicate the various pathways to derive PNEC and the PEC/PNEC comparison. In addition, the Process Maps indicate where:

- The substance is not hazardous (i.e. is of no immediate concern).
- Further data are required.
- There is a need to initiate risk assessment, because use and disposal of the substance are predicted to lead to concentrations which may be harmful.

The Process Maps also alert the user to the possibility of indirect effects of the substance on man and the environment, such as accumulation via food chains.

The following general principles underlay the use of the process maps:

- All relevant physical, chemical and biological data to be used must be reviewed and judged to be of an acceptable quality.
- In general data from lower tiers of the effects assessment are only used if data for the higher tiers are not available.

- Ecosystem studies or field monitoring data, carried out to acceptable standards, provide the best basis for establishing the PNEC (and PEC).
- Depending on the use-pattern of the substance, the development of PECs will be on a local or regional basis but in both scenarios the step-wise phases are recognised: Screening, Confirmatory and Investigative.

The Process Maps (Appendix F) are divided into four parts:

Part 1 provides for an initial assessment of the existing database and considers characteristics of the substance which should have influenced experimental design or warned of the possibility of indirect effects (as distinct from direct toxic effects in the environment).

Parts 2, 3 and 4 are principally concerned with the databases of acute, chronic and ecosystem effects respectively; assessing existing data and indicating if required, what type of additional data are needed.

5.4 ISSUES FOR FURTHER CONSIDERATION

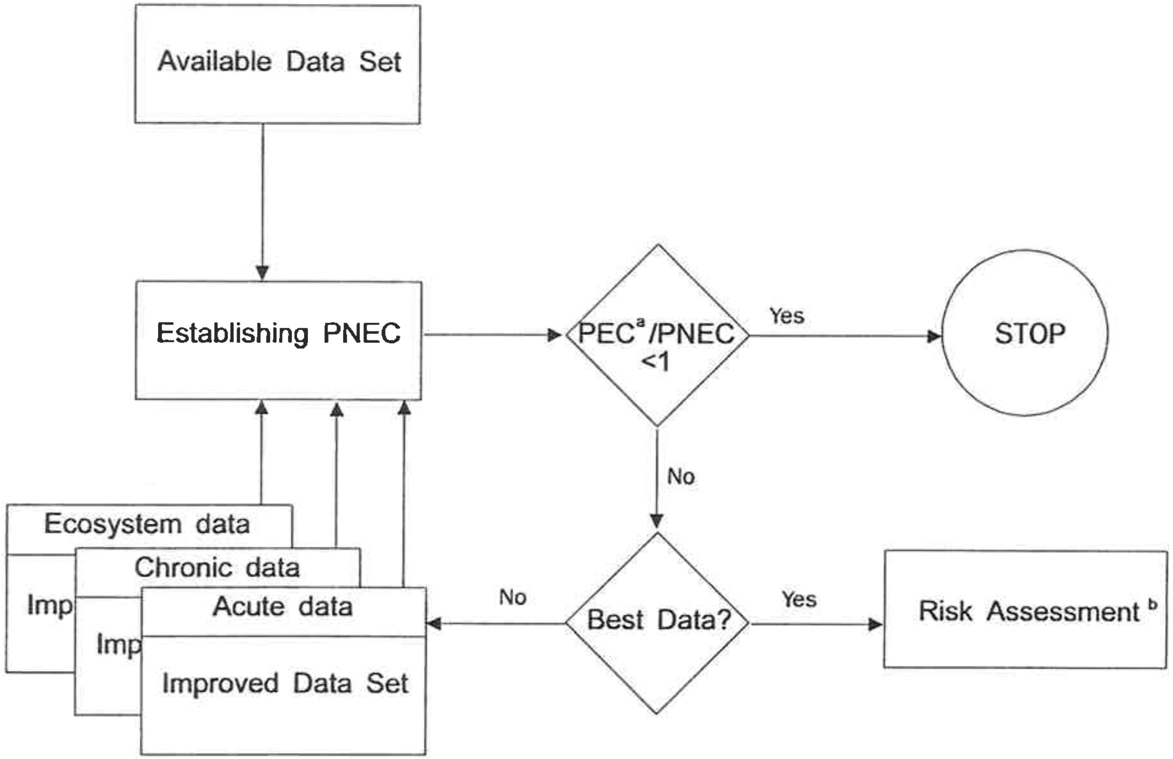
Ecotoxicological data collected in the laboratory can be difficult to translate into accurate predictions of effects that might occur in the field. Some features will tend to make laboratory tests overestimate effects in the field; with other the reverse may be the case.

Observations indicate that laboratory test data more commonly overestimate than underestimate toxicity. The use of laboratory test data will in general lead to an overestimate of toxic effects in the field (and thus lead to very conservative application factors) as a result of the following:

- Laboratory toxicity tests are generally conducted in filtered water of low suspended solids and organic matter content. Bioavailability of substances and therefore their capacity to be toxic tend to be maximised in the laboratory whereas in natural waters concentrations of dissolved organic matter (e.g. humic acids) and suspended solids may reduce bioavailability as a result of complexation or adsorption.

- In laboratory tests rigorous efforts are made to maintain exposure concentrations, whereas, in most field situations exposure will vary over time and rates of degradation are likely to be higher. A paucity of data on how, in practice, concentrations vary in the field has generally led to a conservative approach whereby maximum observed or predicted concentrations are used in hazard assessment with little if any knowledge of the realistic duration of such exposures in the environment. This use of constant concentrations is likely to overestimate hazard, particularly when the results of

FIGURE 4
CONDENSED PROCESS SCHEME EFFECTS ASSESSMENT
(Establishment and Refinement of PNEC)



a Use PEC from Figure 2

b Only if best data for PEC and PNEC were used.

relatively long-term laboratory toxicity studies are the basis for extrapolation.

- We aim to protect populations and communities, rather than individuals but laboratory studies are normally made on individuals and therefore exclude the presence of the homeostatic mechanisms operating in natural ecosystems. This might lead to an overestimation of the effect of the presence of a substance on an ecosystem.

Features of laboratory tests which will generally lead to an underestimate of toxic effects in the field:

- Relatively few species are used to produce laboratory toxicity data and it would be unrealistic to assume that they will encompass the most susceptible species in the field. Also, the disturbance of a fragile equilibrium between species can lead to effects on an ecosystem which could not be predicted from tests on individual species.

- Information on the toxicity of substances to aquatic organisms obtained from laboratory studies usually refers to substances tested singly. However, in natural waters complex mixtures of anthropogenic and natural substances might be present. Examination of the literature on the testing of mixtures shows that for organic substances with a similar mode of action on acute lethal effects are additive (Broderius and Kahl, 1985; Hermens *et al*, 1984). Further information is needed on the effects of mixtures at low concentrations as the literature is conflicting. Alabaster (1981) concluded that toxicant concentrations lower than the NOEC do not contribute to toxicity whilst Hermens *et al* (1984 and 1985) and Deneer (1988) reported that if there is a common mode of action the NOEC of the mixture can be predicted on the basis of additive effects.

- In the laboratory, particularly in longer term tests, efforts are made to optimise conditions for the test organism i.e. remove stressors other than the substance under test. In the field non-chemical stressors, e.g. temperature, concentration of dissolved oxygen or disease may act to increase susceptibility to a substance above that found in laboratory tests.

- The use of a fixed application factor between acute E(L)C50 values and chronic NOECs does not consider the possibility that differences in toxic mechanisms exist between acute and chronic exposure.

Generally it is accepted that appropriate field studies or monitoring data are much more relevant than simple laboratory studies in assessing the hazard associated with the presence of a substance in the environment. However, it should be borne in mind that ecosystem studies/monitoring programmes need to be well designed and carefully executed to enable realistic No Effect values to be obtained. For example,

- the history of the ecosystem in a monitoring study is not always known. Thus an observed 'anomaly' in the ecosystem cannot be attributed with reservation to the presence of substances at the time of monitoring.

The hazard assessment scheme presented here, although intended to cover all compartments, is based almost entirely on data obtained on aquatic organisms. There is a clear shortage of data on soil or sediment organisms, especially on data obtained under relevant and realistic exposure scenarios. The suitability of this paper to address questions on risks to organisms in these compartments associated with the presence of substance substances is therefore uncertain.

SECTION 6. APPLYING THE PROCESS TO CASE STUDIES

This section describes the results of applying the proposed methods for hazard assessment to six substances of differing properties for which a suitable data base was available. The section begins with the determination of PECs and their assessment against monitoring data, lists the extent of our knowledge on the effects of the substances and derives PNECs according to the rules set out in Section 5 and then makes a comparison of the various classes of PEC with the PNECs derived from the various levels of effects data.

6.1. APPLICATION OF MODELS IN EXPOSURE ASSESSMENT

6.1.1. REGIONAL MODELS

The 'PRISEC' model, developed by RIVM (Van de Meent and Toet, 1992), and the 'HAZCHEM' model, developed by ten Berge (1992) based on a recent publication of Mackay *et al* (1992) were employed to test the usefulness of the hazard assessment scheme. For this purpose, six susbtances were selected for which calculations were carried out. In this preliminary test no attempt could be made to collect and screen input data extensively, in particular the emission data are based on rough estimates as described in Section 4.2.1 for the screening phase.

The calculations of the PRISEC and HAZCHEM models cover two scenarios, representing The Netherlands ('NL') and Europe ('EUR'). These scenarios were chosen because PRISEC calculates background concentrations for a European scenario and uses these data as input for the NL scenario calculations.

Comparison of the PRISEC and HAZCHEM models and some measured data for 6 selected substances

The data for the substances were obtained from BUA and RIVM reports, and for LAS the detergent industry supplied additional data. The physico-chemical, environmental and emission data used are listed in Appendices G to I, respectively. Often rough estimates had to be used for model input.

In a first approach the results for a 'Europe' and 'NL' scenario (Table 4) calculated with 'PRISEC' (column 1 and 2) and HAZCHEM (column 3 and 4) were compared as ratios (column 7 and 8) to evaluate the outcome of the models.

Both models show similar results. Differences appear at extremely low concentrations which can be considered as irrelevant. The calculations of the fate of substances in a

WWTP are different in both models. A basic difference is that SIMPLETREAT, used in PRISEC, assumes that biodegradation only occurs in the water phase and therefore in this model the hydraulic retention time is essential. The WWTP model of HAZCHEM is based on Namkung and Rittmann (1987) and also takes the sludge retention time into account. Some other differences for the NL scenario could be explained by the different input concentrations for advection for the compartments. PRISEC calculates average concentrations for the NL scenario, using data from the European calculations. In HAZCHEM no background contribution is assumed in both cases. This aspect of boundary conditions will have to be evaluated further.

To compare the order of magnitude of predicted concentrations with environmental data, figures from actual measurements of the compounds in defined representative sites are needed. These were not readily available, but some field data could be obtained (BUA, ECETOC, 1988). It is obvious that the ranges of concentrations (columns 5 and 6) are very large, since the data represent the largest ranges found in the literature after a first screening. For a first comparison of these rough data the extremes of the measured concentrations (columns 5 and 6) have been divided by the HAZCHEM results for a 'European scenario' (column 3). This means that if the calculated concentration is within the reported range of environmental concentrations, the ratio 'low/HAZ-EUR' (column 9) should be <1 and the ratio 'high/HAZ-EUR' >1 (column 10).

In a number of cases the calculated values were found to be within the measured range. In several other cases, however, the data deviated strongly. For LAS concentrations in water and sediment, DEHP and 3,4-DCA concentrations in sediment and NTA concentrations in water, the predictions were too low. One reason for this deviation may be that the concentrations have been measured near waste water discharges, while the model predicts average concentrations. An explanation for the prediction of low sediment concentrations may be due to unrealistic half-life times for these compartments, e.g. because anaerobic conditions with lower rates have not been included.

Apart from this it must be stressed that reliable data of environmental concentrations in various environmental compartments are seldom available due to selective sampling, but would be essential for validation.

Sensitivity analysis.

In order to evaluate the influence of the variation of different environmental parameters on the outcome of HAZCHEM calculations, a sensitivity analysis for six selected substances has been performed using Monte Carlo simulations. The Monte Carlo simulation is a

TABLE 4

COMPARISON OF CALCULATIONS USING PRISEC AND HAZCHEM MODELS FOR A DUTCH (NL) AND A EUROPEAN (EUR) SCENARIO

Compartment	PRISEC		HAZCHEM		Measured envir. conc.*		PRISEC/HAZCHEM RATIO		low/HAZ-EUR	high/HAZ-EUR
SCENARIO	EUR	NL	EUR	NL	low	high	EUR	NL		
Column No.	1	2	3	4	5	6	7	8	9	10
BZ										
AIR (ug/m3)	2.6	2.8	2.6	$4.8x10^{-1}$	$8.0x10^{-2}$	$1.7x10^{2}$	1.00	5.85	0.03	66.08
WATER (mg/l)	$2.1x10^{-4}$	$2.2x10^{-4}$	$3.9x10^{-4}$	$3.9x10^{-4}$	$1.0x10^{-5}$		0.54	0.56	0.03	2.05
SEDIM (mg/kg)	$6.1x10^{-4}$	$6.8x10^{-4}$	$2.9x10^{-4}$	$2.9x10^{-4}$		$8.0x10^{-4}$	2.10	2.34		
SOIL (mg/kg)	$4.8x10^{-5}$	$4.7x10^{-5}$	$4.5x10^{-4}$	$1.5x10^{-4}$	$4.0x10^{-2}$		0.11	0.31	88.89	
LAS										
AIR (ug/m3)	$8.7x10^{-17}$	$1.4x10^{-16}$	0	$8.6x10^{-15}$			-	0.02		
WATER (mg/l)	$1.1x10^{-3}$	$1.8x10^{-3}$	$6.3x10^{-4}$	$1.0x10^{-3}$	$2.0x10^{-3}$	$7.5x10^{-2}$	1.74	1.77	3.17	118.73
SEDIM (mg/kg)	$6.7x10^{-4}$	$8.8x10^{-4}$	$1.3x10^{-4}$	$2.1x10^{-4}$	1.0	$1.5x10^{2}$	5.19	4.24	7700	$12.0x10^{5}$
SOIL (mg/kg)	$4.1x10^{-2}$	$1.4x10^{-2}$	$1.6x10^{-2}$	$5.4x10^{-3}$	$9.0x10^{-1}$	2.2	2.51	2.57	55.05	134.57
DEHP										
AIR (ug/m3)	$3.5x10^{-3}$	$4.4x10^{-3}$	$1.5x10^{-3}$	$5.5x10^{-4}$	$1.0x10^{-3}$	$3.0x10^{-2}$	2.33	8.00	0.67	20.00
WATER (mg/l)	$5.6x10^{-3}$	$8.1x10^{-3}$	$5.3x10^{-3}$	$4.1x10^{-3}$	$1.0x10^{-4}$	$1.0x10^{-2}$	1.06	1.98	0.02	1.89
SEDIM (mg/kg)	$1.2x10^{-1}$	$1.3x10^{-1}$	$3.5x10^{-2}$	$2.6x10^{-2}$	1.5x10	3.0x10	3.43	5.00	428.57	857.14
SOIL (mg/kg)	$2.9x10^{-4}$	$3.6x10^{-4}$	$2.8x10^{-4}$	$1.0x10^{-4}$			1.04	3.60		

* According to ECETOC (1989); BUA.

TABLE 4 Cntd.

COMPARISON OF CALCULATIONS USING PRISEC AND HAZCHEM MODELS FOR A DUTCH (NL) AND A EUROPEAN (EUR) SCENARIO

Compartment	PRISEC		HAZCHEM		Measured envir. conc.*		PRISEC/HAZCHEM RATIO		low/HAZ -EUR	high/HAZ -EUR
SCENARIO	EUR	NL	EUR	NL	low	high	EUR	NL		
Column No.	1	2	3	4	5	6	7	8	9	10
BHT										
AIR (ug/m3)	$5.3x10^{-3}$	$8.8x10^{-3}$	$4.5x10^{-3}$	$2.4x10^{-3}$			1.18	3.67		
WATER (mg/l)	$7.6x10^{-5}$	$2.0x10^{-4}$	$1.3x10^{-4}$	$1.4x10^{-4}$	$1.0x10^{-4}$	$5.0x10^{-2}$	0.58	1.43	0.77	384.62
SEDIM (mg/kg)	$2.9x10^{-4}$	$6.0x10^{-4}$	$1.5x10^{-4}$	$1.7x10^{-4}$			1.93	3.53		
SOIL (mg/kg)	$2.5x10^{-6}$	$4.2x10^{-6}$	$1.5x10^{-7}$	$8.0x10^{-8}$			16.67	52.50		
DCA										
AIR (ug/m3)	$1.8x10^{-3}$	$2.5x10^{-3}$	$1.0x10^{-3}$	$1.0x10^{-3}$			1.80	2.50		
WATER (mg/l)	$1.5x10^{-3}$	$2.2x10^{-3}$	$1.7x10^{-3}$	$2.3x10^{-3}$	$2.0x10^{-5}$	$4.2x10^{-4}$	0.88	0.96	0.01	0.25
SEDIM (mg/kg)	$6.1x10^{-4}$	$8.7x10^{-4}$	$1.8x10^{-4}$	$2.4x10^{-4}$	$3.96x10^{-2}$	$8.59x10^{-2}$	3.39	3.63	220.00	477.22
SOIL (mg/kg)	$9.6x10^{-6}$	$1.3x10^{-5}$	$2.0x10^{-6}$	$2.1x10^{-6}$			4.52	6.19		
NTA										
AIR (ug/m3)	$4.2x10^{-21}$	$2.6x10^{-22}$	0	0			-	-		
WATER (mg/l)	$2.3x10^{-6}$	$1.5x10^{-7}$	$1.53x10^{-6}$	$2.4x10^{-6}$	$3.0x10^{-4}$	$5.0x10^{-4}$	1.50	0.06	196.23	327.05
SEDIM (mg/kg)	$3.3x10^{-7}$	$1.8x10^{-8}$	$7.12x10^{-8}$	$1.1x10^{-7}$			4.64	0.16		
SOIL (mg/kg)	$9.4x10^{-7}$	$3.1x10^{-15}$	$3.76x10^{-7}$	$1.3x10^{-7}$			2.50	0.00		

* According to ECETOC (1989); BUA.

statistical method for random sampling of input parameters with normal or lognormal distribution patterns. The parameters for which a (log)normal distribution input has been used for LAS are summarised in Appendix J. The essential groups of input parameters for the Mackay level 3 fugacity model consist of

- substance properties,
- discharge characterisation,
- environmental compartment and exchange rates specification.

Most input parameters can vary because of natural variability or inaccuracy in determination. Additive or multiplying effects by a combination of (reasonable) worst case assumptions may give an unrealistic prediction of environmental concentrations.

Applying Monte Carlo simulations will give insight in the variability of the environmental concentrations estimated.

The principal outcome of the simulations are predicted concentrations for eight different environmental compartments, which are presented in Table 5. The normal average, 5 and 95 percentile values are calculated.

The results for LAS are also presented in graphs for suspended matter and dissolved in surface water (Appendix K).

From the results for LAS, it can be concluded that with the variability for the environmental parameters assumed, 90% of the predicted surface water concentrations are between $4.5x10^{-4}$ and $1.2x10^{-2}$ with a normal average of $3.8x10^{-3}$ mg/l.

Future calculations will include also the variability of the substance properties and discharge characteristics not taken into account in the present simulations.

6.1.2. APPLICATION OF LOCAL MODELS

As an example for the application of local models from the screening to the investigative phase of exposure assessment, the emissions of two household substances (LAS, NTA) are given in Appendices L and M. In addition, another example (textile dye) is shown in Appendix N.

For household substances the emission algorithms are simple. It can be reasonably assumed that more than 99% of the release occurs at the use phase, with little to no loss at the production, formulation and processing phases. Simulation of actual waste treatment processes is essential to estimate the emission to water, air, or soil.

TABLE 5
PREDICTED CONCENTRATIONS OF THE SIX SELECTED SUBSTANCES IN THE DIFFERENT ENVIRONMENTAL COMPARTMENTS.

Substance	Compartments (as defined in the model)	Average	5 % <	5 % >
LAS	air (µg/m^3) [a]	3.23×10^{-12}	$<3.0 \times 10^{-13}$	2.08×10^{-11}
	biota (ppm)	5.99×10^{-2}	7.11×10^{-3}	1.95×10^{-1}
	sediment (ppm)	4.90×10^{-3}	3.23×10^{-3}	1.38×10^{-2}
	arable soil (ppm)	4.42×10^{-4}	7.02	$1.11 \times 10^{+2}$
	natural soil (ppm)	0	0	0
	susp. matter (ppm)	3.79	4.49×10^{-1}	1.23×10
	diss. water (mg/l)	3.79×10^{-3}	4.49×10^{-4}	1.23×10^{-2}
	susp. water (mg/l)	7.81×10^{-5}	1.54×10^{-5}	2.16×10^{-4}
DEHP	air (µg/m^3)	2.62×10^{-2}	4.56×10^{-3}	8.95×10^{-2}
	biota (ppm)	$1.58 \times 10^{+2}$	3.26×10	$7.30 \times 10^{+2}$
	sediment (ppm)	2.06×10	2.88	6.49×10
	arable soil (ppm)	8.64×10	2.17×10	$1.75 \times 10^{+2}$
	natural soil (ppm)	5.71	1.75	1.24×10
	susp. matter (ppm)	$3.21 \times 10^{+2}$	7.23×10	$8.95 \times 10^{+2}$
	diss. water (mg/l)	4.15×10^{-2}	8.58×10^{-3}	1.06×10^{-1}
	susp. water (mg/l)	6.70×10^{-3}	2.38×10^{-3}	1.34×10^{-2}
BHT	air (µg/m^3)	4.82×10^{-3}	1.08×10^{-3}	1.34×10^{-2}
	biota (ppm)	1.37×10^{-1}	4.76×10^{-2}	3.01×10^{-1}
	sediment (ppm)	3.50×10^{-3}	3.32×10^{-4}	1.04×10^{-2}
	arable soil (ppm)	2.60×10^{-2}	7.28×10^{-3}	5.59×10^{-2}
	natural soil (ppm)	1.00×10^{-4}	3.48×10^{-5}	2.39×10^{-4}
	susp. matter (ppm)	2.79×10^{-1}	8.25×10^{-2}	6.52×10^{-1}
	diss. water (mg/l)	6.87×10^{-5}	2.39×10^{-5}	1.51×10^{-5}
	susp. water (mg/l)	7.14×10^{-6}	1.35×10^{-6}	1.87×10^{-5}
DCA	air (µg/m^3)	2.42×10^{-4}	6.87×10^{-5}	5.13×10^{-4}
	biota (ppm)	5.95×10^{-3}	5.38×10^{-4}	1.45×10^{-2}
	sediment (ppm)	2.40×10^{-3}	5.38×10^{-4}	8.06×10^{-3}
	arable soil (ppm)	2.68×10^{-4}	6.89×10^{-5}	7.18×10^{-4}
	natural soil (ppm)	2.02×10^{-5}	4.18×10^{-6}	5.84×10^{-5}
	susp. matter (ppm)	1.22×10^{-2}	3.08×10^{-3}	2.82×10^{-2}
	diss. water (mg/l)	1.98×10^{-4}	5.64×10^{-5}	4.80×10^{-4}
	susp. water (mg/l)	3.39×10^{-7}	4.77×10^{-8}	9.72×10^{-7}
NTA	air (µg/m^3) [a]	2.82×10^{-19}	$<3.3 \times 10^{-20}$	9.95×10^{-19}
	biota (ppm)	6.84×10^{-6}	9.02×10^{-7}	2.07×10^{-5}
	sediment (ppm)	8.59×10^{-6}	3.52×10^{-7}	3.31×10^{-5}
	arable soil (ppm)	4.01×10^{-3}	1.08×10^{-3}	7.42×10^{-3}
	natural soil (ppm)	0	0	0
	susp. matter (ppm)	1.91×10^{-3}	2.53×10^{-4}	5.80×10^{-3}
	diss. water (mg/l)	1.37×10^{-5}	1.80×10^{-6}	4.14×10^{-5}
	susp. water (mg/l)	3.85×10^{-8}	9.06×10^{-9}	9.39×10^{-8}
BZ	air (µg/m^3)	2.86	8.53×10^{-1}	7.58
	biota (ppm)	1.89×10^{-3}	8.06×10^{-4}	3.94×10^{-3}
	sediment (ppm)	7.53×10^{-4}	1.67×10^{-4}	2.06×10^{-3}
	arable soil (ppm)	3.69×10^{-4}	8.55×10^{-5}	1.29×10^{-3}
	natural soil (ppm)	6.40×10^{-5}	9.77×10^{-6}	1.92×10^{-4}
	susp. matter (ppm)	4.02×10^{-3}	1.16×10^{-3}	9.25×10^{-3}
	diss. water (mg/l)	2.80×10^{-4}	1.20×10^{-4}	5.85×10^{-4}
	susp. water (mg/l)	1.08×10^{-7}	2.00×10^{-8}	2.95×10^{-7}

[a] These values are not reliable because:

- these values are much influenced by the arbitrary value of the vapour pressure, that was taken extremely low (1.1×10^{-10} Pa) to indicate the low evaporation.
- the low values could not be processed in the HAZCHEM program.

Correspondingly, reliable estimation or measurement of effluent concentrations of waste water treatment plants is a prerequisite to adequate predictions of concentrations in river water. Most river dilution models are simple mass balance models with a single dilution factor, and absence of in-stream removal (i.e. non-reactive substance).

Screening Phase.

Estimation of the likely concentrations of household substances in raw sewage is calculated based on given information on the quantities of the substance used (per capita/day) and data on the per capita flows of wastewater (200 l/cap x day) (Table 6, Appendix L).

TABLE 6

CALCULATION OF PEC AT SCREENING PHASE (General Local Procedure)

Substance	**LAS**
Use pattern - purity - consumption during use - domestic waste water flow	household substance - 100% - specific consumption: 1.66kg/cap x yr with no removal during washing (worst case) - 200l/cap x day
concentration in waste water Model prediction of removal during treatment elimination factor (degradation, sorption, and volatilization) dilution of waste water treatment plant outlet to surface water **generic environmental concentration**	PEC_{ww} = 22.7mg/l 94.8% 19 10 **PEC_{river} = 0.118mg/l**

WWTREAT was used for the estimation of the concentrations in treated sewage effluents and sludges. WWTREAT is a mathematical model which predicts the percent removal and distribution of household substances between air, effluent and sludge for primary and activated sludge waste water treatment plants using experimentally determined distribution coefficients and biodegradation rate constants. At the screening phase, a half-life of 1 day for readily biodegradable substances is used in the WWTREAT model. Model outputs are used to assess the total percentage of removal and percentage of biodegradation of the substance (Appendix M).

A PEC for surface waters is estimated using a dilution factor of 10 for the discharge of treated sewage effluent as mentioned in Section 4.3.1.

Confirmatory Phase.

For the initial application of the local WWTP model, approximate input parameters for sorption and biodegradation are used. Refinement with actual measured sorption coefficients, and experimentally determined rate constants will allow more reliable estimation of the removal (Appendix L). Simulation of the dynamic fate and transformation rates of the substance in representative test systems (e.g. OECD confirmatory simulation tests) will allow further refinement of the chemical input data.

TABLE 7
CALCULATION OF PEC AT CONFIRMATORY PHASE

Substance	**LAS**
Use pattern - purity - consumption during use - domestic waste water flow	household substance - 100% - specific consumption: 1.66kg/cap x yr with no removal during washing (worst case) - 200l/cap x day
concentration in waste water	PEC_{ww} = 22.7mg/l
Removal during treatment (simulation test)	98.6%
elimination factor (degradation, sorption, and volatilization)	71
dilution of waste water treatment plant outlet to surface water	10
generic environmental concentration	**PEC_{river} = 0.032mg/l**

Investigative Phase.

Models are typically developed for specific substances, classes of substances, or environmental compartments. These models embody the current understanding of the substance and the environmental compartment of interest. To ensure accurate predictions, the model results need to be validated by comparing them to laboratory and monitoring data.

In this particular example, measured values of removal are used, because practical experience in the actual environment should carry the greatest weight. Therefore, where data are available from environmental monitoring studies in the receiving environments, these should be used in preference to predictions based on laboratory simulation studies or mathematical models. The monitoring studies must of course be properly designed and employ analytical techniques which are sufficiently sensitive to, and specific for, the substance under study.

TABLE 8

CALCULATION OF PEC AT INVESTIGATIVE PHASE

Substance	**LAS**
Use pattern - purity - consumption during use - domestic waste water flow	household substance - 100% - specific consumption: 1.66kg/cap x yr with no removal during washing (worst case) - 200l/cap x day
concentration in waste water Measured removal during treatment elimination factor (degradation, sorption, and volatilization) dilution of waste water treatment plant outlet to surface water **generic environmental concentration**	PEC_{ww} = 22.7mg/l 99.0% 100 10 **PEC_{river} = 0.023mg/l**
measured environmental concentrations (surface water)	0.005-0.2mg/l

6.2. ESTABLISHING PNECS IN THE CASE STUDIES

6.2.1. ORIGINS OF DATA

For seven of the substances toxicity data were collected for both aquatic and terrestrial organisms. However, emphasis has been placed on the aquatic compartment and no application factors have been proposed yet for the terrestrial environment. For LAS an ECOSOL database (1992) was used: the data were for C12 alkyl chain length or for unspecified alkyl chains. Both laboratory and ecosystem/field data were included. Unlike the data from the AHA database the case-study data were not selected according to pre-determined criteria but they were supplied by ecotoxicologists familiar with the substances.

6.2.2. TREATMENT OF DATA

A database was constructed allowing the entry and analysis of information. Care was taken to eliminate duplicate entries in the database. Rules were applied by which the data could be classified as acute or chronic and, where necessary, could be assumed to belong to the parameters NOEC, LOEC or EC_{50}. Equivocal data were omitted. Appendix D describes the treatment of the data more fully.

6.2.3. AVAILABILITY OF DATA

Appendix D also summarises the amount and type of data available for each substance. The total number of records for a given substance varied from 9 to 380 (mean 110) and the number of species from 8 to 78 (mean 38).

6.2.4. CALCULATIONS

Where the data included more than one study per species for a given end-point (Acute EC_{50} etc) the geometric species mean was calculated for that species. Acute:Chronic, Chronic:Ecosystem and Acute:Ecosystem ratios were calculated and are given in Table 9. Also PNECs were calculated using the Application Factors given in Section 5. These are listed in Table 10.

TABLE 9

RATIOS OBSERVED BETWEEN EFFECTS END-POINTS FOR EIGHT SUBSTANCES

Substance	Acute EC_{50}: Chronic NOEC	Chronic NOEC: Ecosystem NOEC	Acute EC_{50}: Ecosystem NOEC
BHT	131		
BZ	1.31		
CYP	12.7	0.10	1.3
DCA	356	0.93	331
DEHP	1.0		
LAS	6.68	0.61	4.0
NTA	6.28		
Zn	8.59	1.00	8.6

These results indicate that although in the most extreme cases the factor of 40 for predicting the Chronic NOEC from the Acute EC_{50} may not be sufficient, the factor of 200 (Acute EC_{50}:Ecosystem NOEC) is, for three out of four substances 23 to more than 150 times too conservative and for the fourth is a little over 0.6 of the value needed. Dichloroaniline (DCA) is an example of a substance in which a wide variety of acute toxicity results occurs (range: 0.2-80mg/l).

The data shown in Table 10 result from dividing the geometric mean acute EC_{50}s by 200 and the chronic NOEC values by 5 and by taking the observed ecosystem NOECs per se.

TABLE 10
PNECS (μg/l) DEVELOPED FOR EIGHT SUBSTANCES FROM VARIOUS DATA

Substance	PNEC from		
	Acute EC_{50}	Chronic NOEC	Ecosystem NOEC
BHT	320	98	
BZ	240	7300	
CYP	0.0019	0.006	0.29
DCA	46	5.2	28
DEHP	0.67	26	
LAS	23	160	1140
NTA	820	5200	
Zn	16	74	370

They demonstrate a general trend that PNECs predicted from data early in the ecotoxicological hierarchy, i.e. Acute EC_{50} tend to be significantly lower than those from Chronic NOECs (exceptions: BHT, DCA) and lower by an extremely large factor from the Ecosystem NOEC (exception: DCA).

6.3 HAZARD ASSESSMENT

In this section the hazard assessment scheme has been applied for a number of substances. Considering the two aspects of hazard assessment it should be noted that the PNECs so far cover only the aquatic compartment. PNECs for the terrestrial compartment have still to be developed. The PECs have been calculated for the different environmental compartments both for the regional and local situations. The results of HAZCHEM EUROPE have been used in the scheme for the regional model.

A comparison is made between the three tiers of PNECs derived in section 6.2 from acute, chronic and ecosystem studies and the tiers of PECs derived in Section 6.1.

To the extent that the relevant data are available, chronic effect data take precedence over the acute effect data and data from the confirmatory phase take precedence over the data from the screening phase. In the given examples the most reliable PEC/PNEC ratio is marked by double border (Table 11 and Appendix O). Table 11 summarizes the results of the proposed Hazard Assessment process applied to the aquatic compartment on LAS.

TABLE 11

RESULT OF HAZARD ASSESSMENT FOR THE AQUATIC COMPARTMENT ON LAS

PEC/PNEC ratios
Environmental Compartment: Water
Substance: LAS

EFFECT EXPOSURE	ACUTE		CHRONIC		ECOSYSTEM	
LEVEL PHASE	Regional	Local	Regional	Local	Regional	Local
SCREENING	0.027	5.13	0.004	0.74	0.0006	0.1
CONFIRMATORY		1.39		0.2		0.028
INVESTIGATIVE		1.00		0.14		0.02

	ONGOING	FINAL
Status of Hazard Assessment		X

☐ Most reliable PEC/PNEC

The hazard assessment process normally would follow the scheme presented in Section 4.2. For the purpose of the evaluation of the Hazard Assessment process all available data on LAS are presented. The proposed steps in the process would include the Regional/Screening followed by Local/Screening both based on Acute toxicity data.

Based on the PEC/PNEC ratio of 5.13 at the Local/Screening level either data refinement at the Local/Confirmatory level based on acute toxicity data or Local/Screening based on chronic toxicity data could have been the next steps in the hazard assessment. Following the logical approach, the hazard assessment would in the latter case have resulted in a PEC/PNEC ratio < 1. The hazard assessment would then be finished. Based on the additional data presented in the Table it is concluded that further refinement (i.e. moving to the investigative phase and/or to ecosystem toxicological data) is not required for a proper hazard assessment; for illustration the full data set has been included in the Table.

Further examples are included in Appendix O.

SECTION 7. CONCLUSIONS AND RECOMMENDATIONS

It was demonstrated for two compounds that the proposed tiered hazard assessment scheme works for the freshwater environment. From the results, especially on NTA, it is apparent that if the decision criterion "PEC/PNEC < 1" is fulfilled, further refinement of the data does not influence the final judgement and hence is not necessary.

The method is capable of further refinement for other aquatic ecosystems and extension by analogy to other compartments. It is designed to predict the likelihood of directly harmful effects resulting from continuous exposure. Although it is recognised that non-steady-state exposure may be relevant in certain situations, it has not been taken into account in this Report. The assessment of hazard to man caused by substances released into the environment is being studied by another ECETOC Task Force.

The preparation of the method has highlighted the need for further studies in both, exposure and effects assessment. Therefore the following programme is recommended:

Exposure assessment:

- In order to perform further testing of the proposed scheme, additional substances need to be identified covering a broad spectrum of use categories.
- Local release scenarios, with water as the receiving environment, which have been agreed between the competent authorities and industry or which presently are under development, need to be tested within the frame of the hazard assessment scheme, using identified substances.
- Mutually agreed environmental scenarios are required for achieving comparability of results obtained by different institutions. Therefore, standard generic environmental scenarios need to be developed, tested and subsequently proposed for common use.
- Although not all the mechanisms of degradation of substances in the environment are fully understood, a pragmatic approach should be developed for deriving degradation rate constants from the results of standardised laboratory tests. Such rate constants are essential to models designed to predict decomposition of substances in WWTPs or in the environment.
- Some local models, including those for rivers (water/sediment), air and WWTPs need to be selected, tested in the frame of the scheme and finally recommended for use.

- Peak releases of substances into the environment may lead to intermittent exposure. Methods need to be developed for exposure assessment under such non-steady-state conditions.

Effects assessment:

- Long-term studies in the laboratory are considered to be effective predictors of safe concentrations in the natural environment, but the evidence of this would benefit by studies on a wider range than the 13 substances described here.

- Of the few ecosystem data available, the majority originated from the agricultural chemicals industry which were designed to resemble their proposed methods of application. Therefore, they may not equivalently be suited for other substances. Ongoing work in the area of ecosystems (models, field studies) must prove whether the assessment factor holds true for all categories of substances, or whether one type or another must be excluded from this general procedure. The ratios between chronic laboratory and ecosystem studies may be larger or smaller depending on the properties of the substance.

- In this Report, test systems more complex than those of single species were summarised under the term ecosystem, covering a variety of different test designs. More work has to be done to evaluate their design in the aspect of hazard assessment. For example, it is important to define situations when field studies may be essential, desirable or unnecessary. Where they are necessary, criteria for sound studies need to be developed including the suitablitiy of end-points (e.g. ecosystem structure, ecosystem function) and the means of measuring the important parameters. ECETOC will take up this task.

- There is a need for terrestrial ecotoxicology and the study of effects in aquatic sediments to develop in parallel with aquatic ecotoxicology.

- For non-steady-state exposure scenarios there is a special need for studies to develop the principles for coping with these conditions. Principles could include the type of laboratory study and application factors needed.

APPENDICES

APPENDIX A. ENVIRONMENTAL RELEASE OF INTERMEDIATES (Production/Processing)

Reference: BUA Report No.	Substance	Emission (t/a)				Production Volume (t/a)	Emission (% of Production volume)
		Water	Soil	Air	Total		
2	o-Chloronitrobenzene	2.5	-	2.5	5	25,000	0.02
9	o-Nitroanisol	4	-	0.002	4	4,000	0.1
11	m,p-Chloronitrobenzene	16 - 80*	-	-	16 - 80	50,000 - 70,000	0.1
12	Dinitrotoluene	15	-	-	15	125,000	0.01
17	1,2,4-Trichlorobenzene	12	-	-	12	7,000	0.17
23	Tributylamine	< 0.005	-	-	<0.005	500 - 600	<0.001
25	Hexachlorcyclopentadiene	< 0.002	-	<0.005	<0.007	4,000 - 5,000	<0.0002
26	o-Tolidine	0.016	-	<0.05	<0.06	<500	0.01
27	o-Dianisidine	< 0.015	-	<0.007	<0.022	<500	0.004
28	o-Nitroaniline	1.8	-	0.7	2.5	6,000	0.04
32	Benzoldicarbonitrile	1.2	-	-	1.2	1,000	0.1
33	1,1-Dichloroethane	<< 1	-	<0.02	<<1	20,000	<0.005
35	Vinylchloride	25 - 30	-	330	355 - 360	1,500,000	0.02
40	N,N-Diethylaniline	1.6 - 1.7	-	0.32	2	1,200	0.16
41	Nitrotoluene	12	-	>23	>35	72,500	>0.05
42	1-Chloro-2,4-dinitrobenzene	0.43	-	0.01	0.44	3,500	0.01
43	2-Chloro-4-nitroaniline	0.035	-	0.015	0.05	1,500	0.003
44	3-Trifluoromethylaniline	0.06	-	0.006	0.066	1,000	0.007
46	1,3,5-Trichlorobenzene	0.001	-	0.2	0.2	1,000 (Import)	0.02
48	Styrene	-	-	<438	<438	1,200,000	<0.04
51	N-Ethylaniline	< 1.4	-	<0.09	<1.49	400	<0.37
52	1,2-Dichloronitrobenzene	< 0.7	-	0.04	<0.74	14,000	<0.005
55	Chlorotoluidines	0.049	-	-	0.049‡	5,200	0.001
57	o,m-Chloroaniline	2.5 - 3.0	1.4†	-	3.9 - 4.4	4,600 - 6,000	0.1
59	Nitrobenzene	12	-	8	20	200,000	0.01

* 400 t/a from use † worst case assumption for impurity in certain agrochemicals ‡ all Isomeres

APPENDIX B. MEASURED ELIMINATION IN AN INDUSTRIAL WASTE WATER TREATMENT PLANT VERSUS ELIMINATION FACTORS P PROPOSED AT THE ISPRA WORKSHOP

CAS - No.	Substance	% Elimination†	Henry-Constant Pa x m^3/mol	log Pow	log H	Biodegradation Test	Elimination P% Ispra
67-66-3	Chloroform	> 75	440.8	1.97	2.644	not ready	60
108-90-7	Chlorobenzene	> 99	349.6	2.89	2.544	not ready	60
95-73-8	2,4-Dichlorotoluene	> 98	853.0	4.24	2.931	not ready	80
121-69-7	N,N-Dimethylaniline	> 99	6.424	2.31	0.808	not ready	10
106-47-8	4-Chloroaniline	> 98	0.109	1.88	-0.963	ready	60
98-95-3	Nitrobenzene	> 99.9	2.472	1.85	0.393	not ready	10
78-40-0	Triethylphosphate	> 99.9	-	0.80	-	ready	60
126-73-8	Tri-n-butylphosphate	> 99.9	0.533	3.5	-0.273	ready	80
86-57-7	1-Nitronaphthalene	> 98.5	0.121	3.19	-0.917	not ready	60
121-73-3	1-Chloro-3-nitrobenzene	> 97.6	0.453	2.41	-0.344	not ready	10
100-17-4	4-Methoxynitrobenzene	> 99	0.230	2.03	-0.638	not ready	10
71-36-3	n-Butanol	> 99.97	0.564	0.88	-0.249	not ready	60
67-63-0	Isopropanol	> 99	0.818	0.05	-0.087	ready	60
56-23-5	Carbon tetrachloride	> 94	3080	2.83	3.489	ready	90
100-42-5	Styrene	> 99.6	284.7	2.95	2.454	ready	80
28299-41-4	Ditolylether	> 87	15.7	5.3	1.196	not ready	90
100-51-6	Benzyl alcohol	> 99.7	0.035	1.1	-1.456	ready	60
108-69-0	3,5-Dimethylaniline	95	3.283	1.9	0.516	not ready	10
89-98-5	2-Chlorobenzaldehyde	> 98.7	2.577	2.33	0.411	ready	60
108-88-3	Toluene	> 99.8	601.9	2.73	2.780	not ready	60

† Waste Water Treatment Plant (Bayer AG, Leverkusen-Bürrig)

APPENDIX C. DATA REQUIREMENTS FOR A REGIONAL MODEL FOR EXPOSURE ESTIMATION

C.1. PRODUCTION, USE AND DISPOSAL PATTERN OF THE SUBSTANCE

The production volume and the percentage discharge to the air, water and soil and to waste water treatment plants during production, formulation, use and disposal, dependent on use pattern, are necessary data for tracing the discharge routes to the environment.

C.2. PHYSICO-CHEMICAL DATA OF THE SUBSTANCE

The relevant data in this connection are:

- melting point
- molecular weight
- vapour pressure
- water solubility
- octanol-water partition coefficient.

With information on the organic carbon content in the environmental compartments and on the octanol-water coefficient the partition coefficients between the environmental compartments can be estimated.

If the partition coefficients between

- soil/water
- sediment/water
- suspended particulates/water
- biota/water
- primary sludge/water (waste water treatment plant)
- secondary sludge/water (waste water treatment plant)

cannot be derived from the octanol water coefficient because of dissociation in ions, they have to be determined experimentally in the environmental system of interest.

C.3. DATA ON REACTIVITY OR STABILITY OF THE SUBSTANCE

Data on reactivity and stability are mostly entered in the model as kinetic degradation rate constants or as half life times in the air, water, soil or sediment compartments. Very often these data are not available and must be calculated or estimated by expert judgement.

C.4. CHARACTERISTICS OF THE MOSTLY USED WASTE WATER TREATMENT PLANT

If a waste water treatment plant is part of the environmental discharge pathway, the following characteristics of it should be provided like:

- number of inhabitant equivalents discharged
- volume of waste water per inhabitant per day
- concentration of primary sludge
- organic carbon content of primary sludge
- concentration of sludge in aeration tank
- organic carbon content of sludge aeration tank
- hydraulic retention time
- sludge retention time
- biodegradation rate from experimental tests

C.5. CHARACTERISTICS OF THE REGIONAL ENVIRONMENT

The predicted exposure levels are dependent on the specific properties of the environment of interest like:

- temperature
- total surface area
- percentage surface of water
- percentage of arable land and pasture
- percentage of forests and woodland
- height of air compartment
- depth of soil and sediment compartments
- concentration of organic carbon in soil, sediment and suspended sediment. On the basis of this information and of the octanol-water coefficient the partition coefficients of the substance between compartments may be estimated.
- advection residence time of air
- advection residence time of water

A sensitivity analysis of the choice of the above parameters is recommended in order to get some feeling of the influence of the environment on predicted environmental exposure concentrations in the EC member states.

C.6. MASS TRANSFER FACTORS (KINETIC PARAMETERS) DESCRIBING THE EXCHANGE PROCESSES BETWEEN THE ENVIRONMENTAL COMPARTMENTS

The mass transfer factors describe the exchange between the environmental compartments air, water, soil and sediment. Mostly these variables are kept fixed values. Mackay (1991) describes the experimental determination of these mass transfer factors for apolar (lipophilic) compounds. The following mass transfer factors (MTC) are relevant:

- air side air/water MTC
- water side air/water MTC
- rain rate
- aerosol deposition velocity
- air side air/soil MTC
- soil air phase diffusion MTC
- soil water phase diffusion MTC
- sediment water diffusion MTC
- suspended particle settling velocity. This settling velocity and the concentration of suspended sediment in water control the sediment deposition velocity.
- resuspension rate of deposited sediment (mm/year). The difference between sediment deposition and resuspension determines the so-called burial rate.
- soil water runoff rate
- soil solids runoff rate.

APPENDIX D. DERIVATION OF APPLICATION FACTORS

D.1 INTRODUCTION

Application factors by which limited data bases can be used to estimate NECs (as described in Section 5.2 and tested in Section 6.2) were derived from the high-quality data base of the ECETOC Aquatic Hazard Assessment (AHA) Task Force (Report in preparation). Additional data were provided from the agricultural chemicals industry to supplement the information on chronic laboratory and ecosystem studies. This Appendix describes methods of analysis and provides tabulations of data from which the summary ratios given in the main text were derived. (Appendix E provides the data used in the case studies to test the realism of the application factors developed here.)

D.2. ACUTE L(E)C$_{50}$:CHRONIC NOEC

D.2.1. METHODS

Various relationships were examined, using data selected in the following manner.

- A general relationship between acute EC$_{50}$ and chronic NOEC was sought, e.g. 'fresh and saline water, all species, all types of substance' using data-selection and SAS programmes. This gave a print-out of the weighted regression line, describing the relationship, listed the raw data used and the number of data entries available on the two axes for each substance.

- A second programming step calculated the ratio (in this case Acute EC$_{50}$:Chronic NOEC) from the geometric means and ranked the substances in ascending order of their ratio, assigning to each a 'Hazen percentile'. This percentile is given for the nth substance as

$$\frac{100}{2x} + \frac{100(n-1)}{x}$$

where x is the total number of substances in the analysis. Thus, if these are ten substances in the series the ones with the lowest (n = 1) and highest (n = x) ratios will be assigned, respectively:

$$\frac{100}{2x10}+\frac{100(1-1)}{10}=\frac{100}{20}= \text{the } 5\%\text{-ile}$$

and

$$\frac{100}{2x10}+\frac{100(10-1)}{10}=\frac{100}{20}+\frac{900}{10}= \text{the } 95\%\text{-ile}$$

This simply creates a symmetrical plot for the cumulative distribution of the ratios as their percentiles, avoiding the statistical improbability of 0% or 100%.

- The data were then checked to ensure that all the substances had more than single data entries on both axes (although, for convenience, a single entry on just one axis was permitted).

- The 90%-ile, i.e. the ratio greater than or equal to 90% of the substances for which data were available, was interpreted logarithmically where an exact 90%-ile was not recorded.

  It was considered that the 90%-ile offered sufficient safety for use in predicting Chronic NOEC values from Acute EC_{50}s. It will, of course, prove conservative in 90% of cases, if the assumption holds that the AHA database selections are representative of all substances. It was realised that the analysis could include substances already known to demonstrate very large acute:chronic ratios (e.g. most heavy metals). Conversely there will be substances where it is known that concentrations giving chronic toxicity are likely to be very close to acute levels, perhaps due to the metabolism and detoxification of the substance within the target organism. In such cases the user may adopt a different approach: otherwise, the 90%-ile is to be the default value for the acute:chronic ratio.

- From the above argument, the heavy metals, organo-metals and inorganic substances could be deleted from each ranked series of ratios and the percentiles recalculated using the smaller number of the remaining substances.

In the accompanying Tables the choice has been given. Tables D-1 (a)-(f) are based on various environments and taxonomic groups but use only organic substances, excluding the organo-metals.

D.2.2. RESULTS

The results are set out in Tables D-1 (a) to (f). The rank order is reversed so that the substance with the highest ratio is given first, then sufficient contiguous ratios until the 90%-ile can be determined, then selections of the data every 5 or 10 entries and finally the substance with the lowest ratio.

The names of the substances are not listed.

N.B. Acute:Chronic ratios of less than 1.0 arise from the way in which the AHA data base is assembled. An acute EC_{50} (geometric mean) may be derived from studies with species different from the geometric mean of the Chronic NOEC. If the species used in the EC_{50} were rather sensitive and those used in the NOEC were rather tolerant the expected acute > chronic value can be overturned.

Selection of the 90%-ile has eliminated the effects of the few substances with exceptionally large Acute:Chronic ratios. Apart from the active ingredients (90%-ile: 48.9) the 90%-ile values rarely much exceed 30, especially where a useful number of substances (>30) was available. Only a handful (4 or 5) substances exceeded the ratio of 50 in any of the selections.

D.2.3. CONCLUSIONS

A practicable 90%-ile Acute EC_{50}:Chronic NOEC value of close to 30 could be justified on the basis of the AHA data. However, for additional safety it is proposed to adopt the factor 40 to predict a Chronic NOEC from an Acute EC_{50}, given that the acute value is the lowest of at least three figures obtained from studies on a minimum of two major taxonomic groups.

D.3. CHRONIC NOEC:ECOSYSTEM NOEC RATIOS

D.3.1 INTRODUCTION

The AHA data base provided information on only three substances. To these, ten active ingredients of agrochemicals were added. The lowest NOECs were taken from both chronic studies in the laboratory and ecosystem studies. Where several results were available for the same species and end-point the geometric mean was calculated and assessed to see whether it represented the lowest NOEC. The ratios were ranked in the same way as with the acute:chronic ratios and the 90%-ile was interpolated using the assumption that the ratios were logarithmically distributed.

D.3.2. RESULTS

Table D-2 shows the individual percentiles and ratios. The median ratio was 1.12 and for six of the active ingredients of agrochemicals the laboratory-derived Chronic NOEC was at or below the Ecosystem NOEC. This result was not altogether surprising. Bioavailability (see Section 5.4) is known to be maximal under laboratory conditions which may add to the stress caused by the toxicant.

The 90%-ile for all thirteen substances was 5.1 but for the active ingredients of agricultural substances alone it was 1.43. However, as studies on such substances are not carried out under steady-state conditions, the ratio Chronic:Ecosystem NOEC may underestimate their toxicity when constant prolonged exposure is achieved.

D.3.3. CONCLUSION

Since active ingredients of agrochemicals may be representative of any substance which has been carefully studied in the laboratory and the field, the 90%-ile ratio for all 13 substances should be adopted for the time being as the factor by which the Chronic NOEC from a laboratory study should be divided to estimate the Ecosystem NOEC. For convenience the factor is rounded to 5.

TABLE D-1
DERIVATION OF ACUTE:CHRONIC RATIOS

Substance Ranking Order	Ratio Acute EC_{50}:Chronic NOEC	Hazen Percentile (See D.2.1.)	Interpolated Ratio for 90% of Substances (90%-ile)
A. Fresh & saline water, all species, organics excluding organo-metals			
58	668	99.1	
57	381	97.4	
56	82.5	95.7	
55	62.4	94.0	
54	45.8	92.2	
53	30.1	90.5	)
52	25.1	88.8	) 28.5
51	24.5		
50	24.3		
45	18.7		
40	14.4		
30	6.4		
20	4.5		
10	2.3		
5	2.0		
1	0.1		
B. As A but fresh water only			
46	668	98.9	
45	82.5	96.7	
44	62.4	94.6	
43	48.9	92.4	
42	30.1	90.2	)
41	26.5	88.0	) 29.7
40	25.1		
35	23.7		
30	14.1		
20	6.5		
10	3.6		
5	2.3		
1	0.1		

TABLE D-1 (cntd.)
DERIVATION OF ACUTE:CHRONIC RATIOS

Substance Ranking Order	Ratio Acute EC$_{50}$:Chronic NOEC	Hazen Percentile (See D.2.1.)	Interpolated Ratio for 90% of Substances (90%-ile)
C. As B but fish & invertebrates only			
45	668	98.9	
44	82.5	96.7	
43	62.4	94.4	
42	48.9	92.2	
41	30.1	90	= 30.1
40	26.5		
35	23.8		
30	14.6		
20	7.8		
10	3.6		
5	2.5		
1	0.7		
D. As C but invertebrates only			
5	40.1	90.0	= 40.1
4	31.3	70.0	
3	21.5	50.0	
2	6.1	30.0	
1	4.8	10.0	
E. As D but fish only			
33	82.5	98.5	
32	62.4	95.5	
31	43.5	92.4	)
30	29.1	89.4	) 31.6
25	23.2		
20	12.6		
10	4.6		
5	2.9		
1	2.0		
F. As A but saline water only			
14	59.0	96.4	)
13	24.5	89.3	) 26.7
12	18.7		
11	13.3		
10	6.1		
5	2.1		
1	0.7		

TABLE D-2
DERIVATION OF CHRONIC NOEC(LABORATORY):ECOSYSTEM

Substance Ranking Order	Ratio Laboratory NOEC:Ecosystem NOEC	Hazen Percentile (See D.2.1.)	Interpolated Ratio for 90% of Substances (90%-ile)
13	6.30	96.15	)
12	4.86	88.46	) 5.12
11*	1.56	80.77	
10*	1.32	73.08	
9*	1.32	65.38	
8	1.22	57.69	
7*	1.12	50.00	
6*	1.00	42.31	
5*	0.70	34.62	
4*	0.33	26.92	
3*	0.33	19.23	
2*	0.12	11.54	
1*	0.10	3.85	

* active ingredient of an agrochemical

APPENDIX E. CONFIRMATION OF APPLICATION FACTORS

E.1. INTRODUCTION

This appendix summarises the effects data base used as an independent check on the application factors derived from the AHA data base. Eight substances were selected for inclusion in the case studies. A large amount of toxicity data was expected to exist on them. They were:

- Linear alkylbenzene sulphonate (LAS)
- Nitrilotriacetic acid (NTA)
- 3,4-Dichloroaniline (DCA)
- Benzene (BZ)
- Diethylhexylphthalate (DEHP)
- 2,6-Di-tert-butyl-4-methylphenol (BHT)
- Cypermethrin (CYP)
- Zinc (Zn)

Toxicity data were collected both for aquatic and terrestric organisms. For LAS, the ECOSOL (1992) database was used (data for LAS-C_{12} or unspecified). Data from ecosystem studies or field tests were included as well. The data were not evaluated according to a uniform set of quality criteria; however, they were supplied by toxicologists familiar with the specific substances.

E.2. TREATMENT OF THE DATA

The following section lists the more important definitions used.

Acute toxicity tests were defined by their duration (a test animal can survive unfed without harm) as follows:

For algae	≤24h
For *Daphnia sp.*	≤48h
For other invertebrates	≤96h
For fish	≤7d

A distinction was made between acute EC_{50} (and LC_{50}), chronic $E(L)C_{50}$ and chronic NOEC. All effects were taken as equally important (lethal and other effects). Unless NOEC, LOEC and EC_{50} were specifically given, partial effects were clustered as follows:

- ECx, $x \leq 16$ ---> NOEC
- ECx, $16 < x \leq 25$ ---> LOEC
- ECx, x is not defined ---> LOEC
- ECx, $25 < x < 84$ ---> EC_{50}
- EC100, LC100, LC90 etc. were not included in the calculations.

  e.g. LC(85%) not included, but
  LC(28%) ---> LC50
  EC(83%) 21d reprod. inhib. *Daphnia*, BHT ---> EC_{50}
- LOEC/2 = NOEC
- NOEC, etc '>' .. or '<' .. ---> not included for calculations
- NOEC, etc '≥' .. or '≤' .. ---> interpreted as '=' ...
- MATC x ½√2 = NOEC

Some authors reported many endpoints from one experiment, e.g. LC_{50} for 4, 7, 14, 28 days, EC_{50} and NOEC at the same observation times. As these data were not independent of each other, they were not all included when correlations or ratios are calculated. For each experiment, only one entry was included as the final test result. This, however, was not always clear. The data in the acute set were independent of the data in the chronic sets. For the acute list of data, the lowest EC_{50} was selected; in most cases this was the result after the longest exposure time. For chronic lists (NOEC and EC_{50}), the endpoint for the most sensitive parameter was used.

E.3. QUANTITATIVE ANALYSIS OF THE DATA

The total number of records in the raw data base varied from 9 for BHT, to 160 for Zn and to 380 for LAS. The total number of species in the data base varied from 8 for BHT, to 78 for Zn and 75 for LAS.

Table E-1 gives an overview of the variation of the number of species, amount of information (records) and the distribution between acute and chronic tests. The number of records referring to a more or less standard test set is also included: algae (all species), *Daphnia* (spec.), fish (all species).

Various calculations were performed with the data in the three lists. When the list contained more than one experiment per species, a geometric mean was calculated for the particular species. For each substance, the mean acute or chronic toxicity was calculated for all species (geometric species mean, one per list). The results of these calculations are presented in Table E-2. These species-means can be compared to the highest and lowest test result (record) per substance and to the 95-(left) percentile of the geometric species-means, calculated according to Aldenberg and Slob (1991).

E.4. CALCULATION OF VARIOUS APPLICATION FACTORS

With the figures presented in Table E-2, application factors have been calculated. The results are presented in Table E-3.

TABLE E-1
AVAILABILITY OF DATA IN THE DATA BASE (NUMBER OF RECORDS)

	BHT	DCA	DEHP	CYP	BZ	NTA	Zn	LAS
Total, m	**9**	**124**	**18**	**41**	**127**	**21**	**158**	**380**
Species, n	8	32	9	26	63	14	78	75
FW Algae	2	6	0	0	9	0	0	31
Daphnia	1	30	8	3	17	5	7	101
Fish	4	40	6	13	37	4	74	174
Marine	0	34	3	10	36	0	52	34
ACUTE, m	**4**	**50**	**5**	**40**	**106**	**15**	**120**	**283**
Species, n	4	17	4	26	52	12	73	57
FW Algae	0	0	0	0	3	0	0	0
FW Daphnia	0	17	2	3	17	2	7	75
FW fish	3	19	2	12	35	2	47	147
Marine	0	6	0	10	29	0	45	30
CHRONIC, m	**5**	**74**	**13**	**1**	**21**	**6**	**38**	**97**
Species, n	4	21	7	1	15	3	20	32
FW Algae	2	6	0	0	6	0	0	31
ECOSYSTEM*	**0**	**3**	**0**	**6**	**0**	**0**	**6**	**12**

* Includes multi-species studies
m = number of records
n = number of species

TABLE E-2
STATISTICAL ANALYSIS OF THE DATA (conc. in mg/l)

	BHT	DCA	DEHP	CYP	BZ	NTA	Zn	LAS
Geom. mean of all acute records	64.41	5.32	0.133	0.63x10^{-3}	34.68	182.21	3.03	5.03
Geom. mean of all chronic records	0.49	0.036	0.136	0.03x10^{-3}	30.52	26.02	0.30	0.81
Ac. E(L)C_{50}, geom. mean	64.41	9.26	0.133[1]	0.38x10^{-3}	47.92	163.53	3.18	4.61
m/n	4/4	50/17	1/1	40/26	106/52	15/12	120/73	283/57
95%-ile, 50% confid.		0.542		2.08x10^{-6}	2.06	39.0	0.189	0.210
95%-ile, 95% confid.		0.118		2.37x10^{-7}	0.888	14.9	9.89x10^{-2}	0.010
highest test result	100	79	>1.00	0.37	600	1000	750	270
lowest test result	0.6	0.19	0.133	5x10^{-6}	0.0058	79.0	0.004	0.013
Chron. E(L)C_{50}, geom. mean	2.81	1.06	0.69	-	47.46	212.78	5.62	5.53
m/n	3/3	41/19	1/1	0/0	8/7	4/2	19/11	32/14
95%-ile, 50% confid.		3.22x10^{-2}			1.03		0.444	0.279
95%-ile, 95% confid.		5.51x10^{-3}			2.1x10^{-2}		0.081	0.045
Chronic NOEC geom. mean	0.49	0.026	0.13	0.03x10^{-3}	36.58	26.02	0.37	0.69
m/n	2/2	33/12	12/6	1/1	13/10	2/2	19/12	65/24
95%-ile, 50% confid.		9.59x10^{-4}	1.46x10^{-2}		1.09		4.19x10^{-3}	0.035
95%-ile, 95% confid.		1.05x10^{-4}	1.15x10^{-3}		7.29x10^{-2}		2.09x10^{-4}	0.009
highest test result	6.6	18.0	>1.0	1.20x10^{-3}	64.0	650	43.2	90
lowest test result	0.05	0.0016	0.024	0.03x10^{-3}	0.053	24	0.01	0.025
Standard species geom. mean ac. LC_{50}	22.6	6.9	0.133	0.004	97.6	99.4	2.1	4.5
Daphnia geom. mean ac. LC_{50}		1.3	0.133					6.54
Daphnia geom. mean chron. NOEC		0.006	0.10					1.04
Field tests NOEC geom. mean		0.028		2.9x10^{-4}			0.37	1.14
number of tests		3		6			6	13
lowest test result		0.015		3x10^{-5}			1.7x10^{-3}	0.09

[1] DEHP: Value for the only test result below the solubility limit.
Some ten other L(E)C_{50} test results were above the solubility limit of 0.34mg/l.

m = number of records
n = number of species

TABLE E-3
CALCULATION OF VARIOUS APPLICATION FACTORS AND PRECENTILES FOR EACH SUBSTANCE

	BHT	DCA	DEHP	CYP	BZ	NTA	Zn	LAS
Acute EC_{50}/Chronic EC_{50}	23.0	8.8	0.2		1.0	0.8	0.6	0.8
Acute EC_{50}/Chronic NOEC	131.5	356	1.0	12.7	1.3	6.3	8.6	6.7
50%-ile	98	433	1.8		1.6	5.4	10	6.3
90%-ile	2692	10180	2.7		37	21	343	130
stand. spec. 50%	16	363	4		2.7	3.9	7.1	6.4
stand. spec. 90%	589	4677	6.2		50	8.9	132	79
Acute EC_{50}/Field NOEC		331		1.3			8.6	4.0
50%-ile				0.7				
90%-ile				102				
Chronic EC_{50}/Field NOEC		38					15	4.9
Chronic NOEC/Field NOEC		0.9		0.1			1.0	0.6
50%-ile		0.7					0.2	0.6
90%-ile		15					186	9.9

APPENDIX F. PROCESS SCHEME - EFFECTS ASSESSMENT

The four process maps which follow (Fig. A6-1 to A6-4) should be used in conjunction with the explanatory notes on the facing pages. They are structured so that the process of hazard assessment can begin at the earliest opportunity but if data are insufficient there is guidance on the most effective means by which the data should be gathered. Thus the map in Part 1 can be used with a full existing data set; Part 2 uses ecosystem studies, Part 3 chronic data and Part 4 acute studies. At each stage there are questions concerning indirect effects resulting from the presence of the substance in the environment and in Parts 2-4 there is an indication of the need for discussions on the management of the risk.

The table in Note (5) (Part 1) referred to in Note (10) (Parts 2-4) was derived from a special study made by the ECETOC Aquatic Hazard Assessment Task Force.

PROCESS MAPS EFFECTS ASSESSMENT EXPLANATORY NOTES, PART 1

(1) The physical/chemical measurements are used in designing (or checking the design of) the experimental studies, for example to confirm that the substance was in true solution or would not have volatilised significantly during the study. Data on analogous substances may aid experimental design or provide an indication of the properties of the specific substance. Similarly QSARs may be examined although they are of lower value in the ecotoxicological hierarchy than actual measurements. Validated QSARs are acceptable if the substance can be assessed by interpolation of the series or matrix making up the QSARs. As well as helping to predict effects QSARs can be used to aid experimental design.

(2) Indirect effects include the transfer of substances via food webs to other target organisms if the primary effects on a species include bioaccumulation. Therefore predictions of bioaccumulation using measured or calculated octanol/water partition (log P) coefficients are required. If measurements of bioaccumulation are available these may be used. Other indirect effects include for example eutrophication or increasing biochemical oxygen demand.

(3) Bioavailability is a complex feature combining attributes of the **substance** and the **environment** in ways which affect the physical or chemical form of the substance.

(4) Determinants used during exposure assessment may identify compartments which the substance may enter. Toxicity testing appropriate to those compartments would then be carried out.

(5) The question is related to the extent of relevant testing. Where this is limited, a very cautious attitude must be taken in deriving PNEC. The value to which an assessment factor should be applied to derive PNEC will be the lowest in a given relevant data set, except that where a number of measurements for the same species and end-point are available the geometric mean may be taken. The value used must be appropriate to the environmental compartment under consideration.

Examples of the availability of data and the corresponding application factors for deriving the PNEC are given below. These factors may be different for each environmental compartment, and particularly the water column rather than aquatic sediments. For active ingredients of agrochemicals there are useful data for terrestrial ecosystems.

Application Factors for Steady-State, Long-Term Exposure

Factors by which given EC_{50} or NOEC should be divided to give PNEC	
Lowest of three EC_{50} values from short-term tests on at least two major* taxonomic groups	200
Lowest NOEC value from long-term tests on at least two major taxonomic groups	5
NOEC value from a model ecosystem study	1

* For example, fish, crustacean, insect, annelid, mollusc, alga, higher plant

(6) Even at this stage the data on the substance or the result of comparing the Predicted or Measured Environmental Concentration (PEC) and Predicted No-Effect Concentration (PNEC) or observations made in the field may indicate that there is no significant risk from manufacture, transport, use or disposal.

(7) 'Acceptable' in this context means that in the light of expert judgement* the studies were carried out and reported in such a manner that it is clear that the science was right and the conclusions were fully supported by the data. Good Laboratory Practice helps here but is not essential.

* Expert judgement may be provided by the notifier of a new substance or the manufacturer of an existing substance, the regulatory authority or an 'outside' expert (eg academic) with relevant knowledge of the particular area.

(8) For new and existing substances, studies could be carried out in model ecosystems. For existing substances the ecosystem study could be a monitoring exercise. The scale and complexity of these systems would be decided on a case by case basis.

(9) Chronic and sub-chronic studies are to be considered together in this stage. Definitions of acute, sub-chronic or chronic exposure have been agreed in ECETOC (ECETOC AHA TF Report, in preparation). These definitions apply more easily to animals than to plants or micro-organisms.

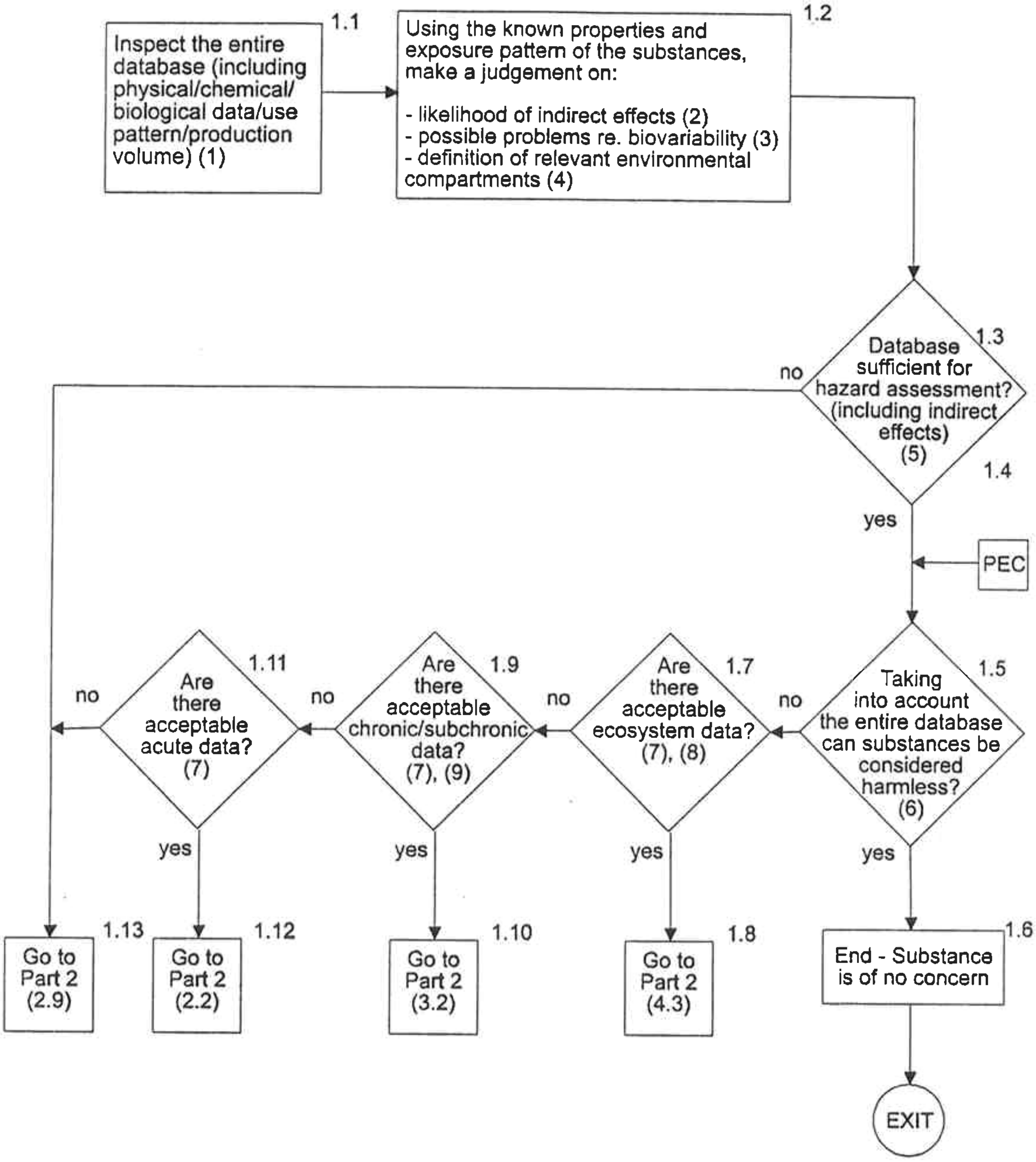
'Acute test' means a test of such short duration that an animal can survive unfed without harm during the period.

'Sub-chronic' means longer than acute exposure but not more than a period equivalent to one third of the time taken to reach sexual maturity.

'Chronic' means longer than sub-chronic.

For the process map, the word 'chronic' includes sub-chronic.

FIGURE F-1
PROCESS MAPS EFFECTS ASSESSMENT, PART 1: INSPECTION OF THE ENTIRE DATA BASE



PROCESS MAPS EFFECTS ASSESSMENT EXPLANATORY NOTES, PART 2

(10) The list in Note (5) gives the factors to be applied to observed toxicity values to calculate the PNEC. In acute studies the EC_{50} may be appropriate. In chronic studies the NOEC should be used.

(11) Since the PNEC derived in these process maps incorporates application factors, a PEC/PNEC ratio of less than 1.0 gives no cause for concern. If the PEC/PMEC is greater than 1.0 further consideration is required. Refinements of the PNEC could include the use of more relevant species, life stages, testing media or exposure conditions (pattern and duration of exposure) thus possibly resulting in a decrease in the application factor. For example if the PEC relates to constant exposure but the actual pattern of exposure is not constant, or if the PNEC is derived from studies where bioavailability of the substance was high but under realistic conditions the substance may be chelated, adsorbed etc then a PEC/PNEC exceeding 1.0 may not result in a problem.

(12) The other properties to be considered here are those related to indirect effects (Note 2).

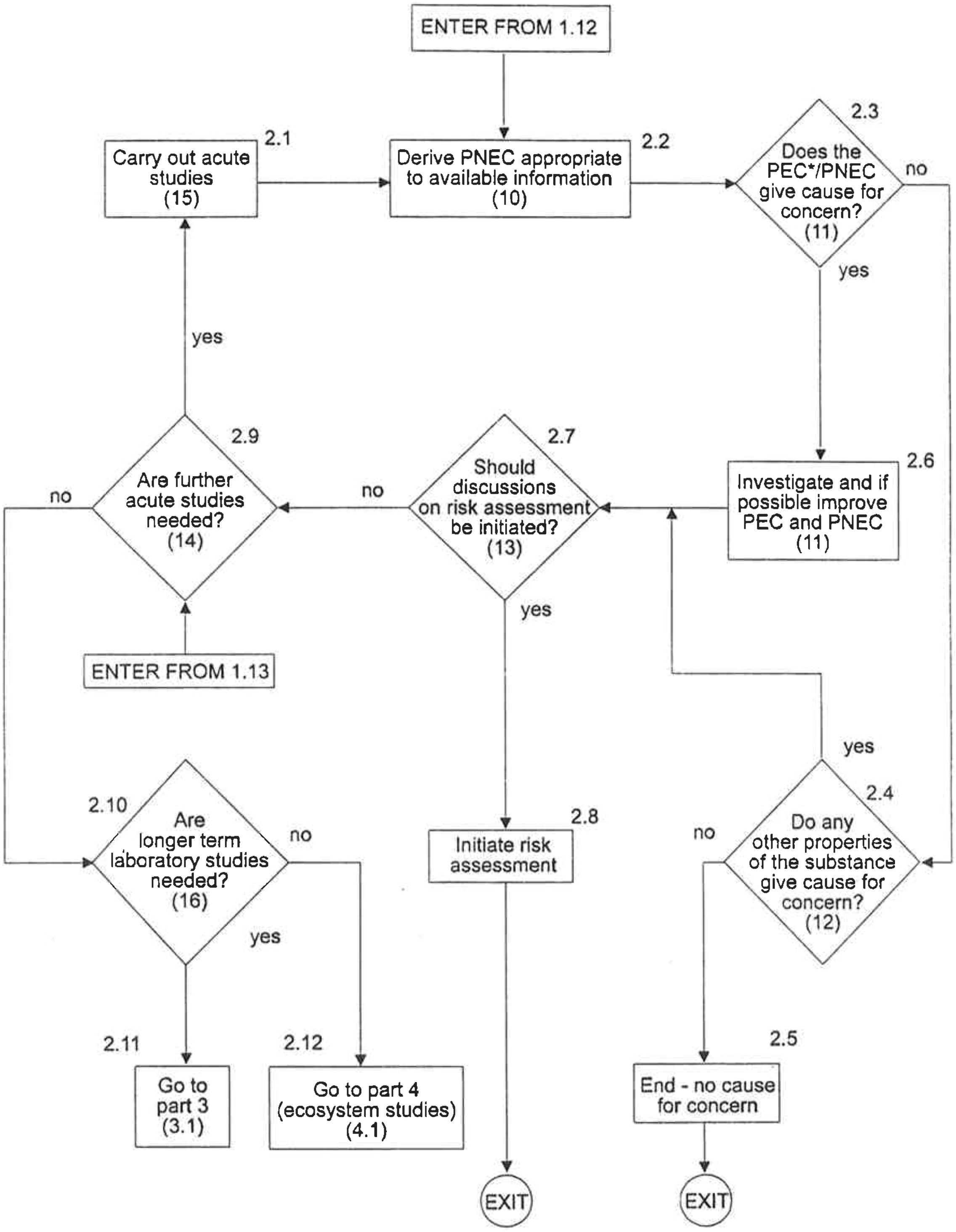
(13) These discussions might be appropriate where it is considered that there is little more to be gained by further testing or the level of concern is such that there is not sufficient time to wait for the extra studies.

(14) The answer 'Yes' will be given where it is more appropriate to carry out further short-term studies to improve that aspect of the data-set than to move to longer-term studies. For example it may be desirable to include a short-term study on an alga or sediment-dwelling invertebrate rather than to examine the effects of the substance on the rate of growth of fish. In other cases, the volatility of a substance may suggest the need for further short-term studies and the irrelevance of longer-term tests.
Similarly, where the initial database indicates large differences between the response of species it may be more useful to study further species in acute exposure.

(15) An inspection of the exposure scenarios and PEC for each environmental compartment will indicate where attention should be focused.

(16) Longer-term studies may be needed where continued exposure is indicated.

FIGURE F-2
PROCESS MAPS EFFECTS ASSESSMENT, PART 2
THE USE OF ACUTE STUDIES



* also measured environmental concentration

PROCESS MAPS EFFECTS ASSESSMENT EXPLANATORY NOTES, PART 3

(10) The list in Note (5) gives the factors to be applied to observed toxicity values to calculate the PNEC. In acute studies the EC_{50} may be appropriate. In chronic studies the NOEC should be used.

(11) Since the PNEC derived in these process maps incorporates application factors, a PEC/PNEC ratio of less than 1.0 gives no cause for concern. If the PEC/PNEC is greater than 1.0 further consideration is required. Refinements of the PNEC could include the use of more relevant species, life stages, testing media or exposure conditions (pattern and duration of exposure) thus possibly resulting in a decrease in the application factor. For example if the PEC relates to constant exposure but the actual pattern of exposure is not constant, or if the PNEC is derived from studies where bioavailability of the substance was high but under realistic conditions the substance may be chelated, adsorbed etc then a PEC/PNEC exceeding 1.0 may not result in a problem.

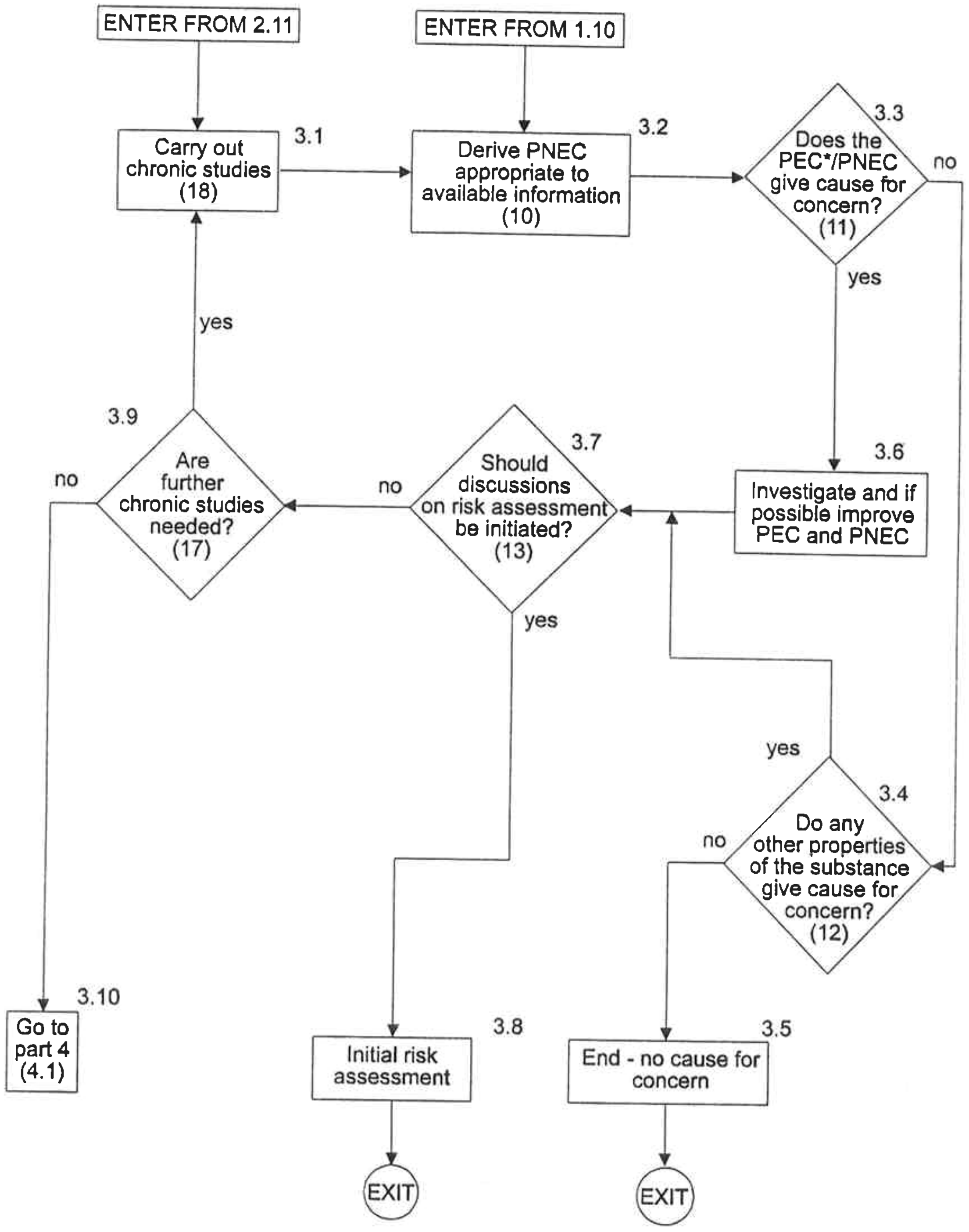
(12) The other properties to be considered here are those related to indirect effects (Note 2).

(13) These discussions might be appropriate where it is considered that there is little more to be gained by further testing or the level of concern is such that there is not sufficient time to wait for the extra studies.

(17) The answer 'Yes' will be given where it is more appropriate to carry out further chronic studies in the laboratory to improve that aspect of the data-set.

(18) See (17). An inspection of the exposure scenarios and PEC for each environmental compartment will indicate where attention should be focused.

FIGURE F-3
PROCESS MAPS EFFECTS ASSESSMENT, PART 3
THE USE OF CHRONIC/SUBCHRONIC STUDIES



* also measured environmental concentration

PROCESS MAPS EFFECTS ASSESSMENT EXPLANATORY NOTES, PART 4

(7) 'Acceptable' in this context means that in the light of expert judgement* the studies were carried out and reported in such a manner that it is clear that the science was right and the conclusions were fully supported by the data. Good Laboratory Practice helps here but is not essential.

* Expert judgement may be provided by the notifier of a new substance or the manufacturer of an existing substance, the regulatory authority or an 'outside' expert (eg academic) with relevant knowledge of the particular area.

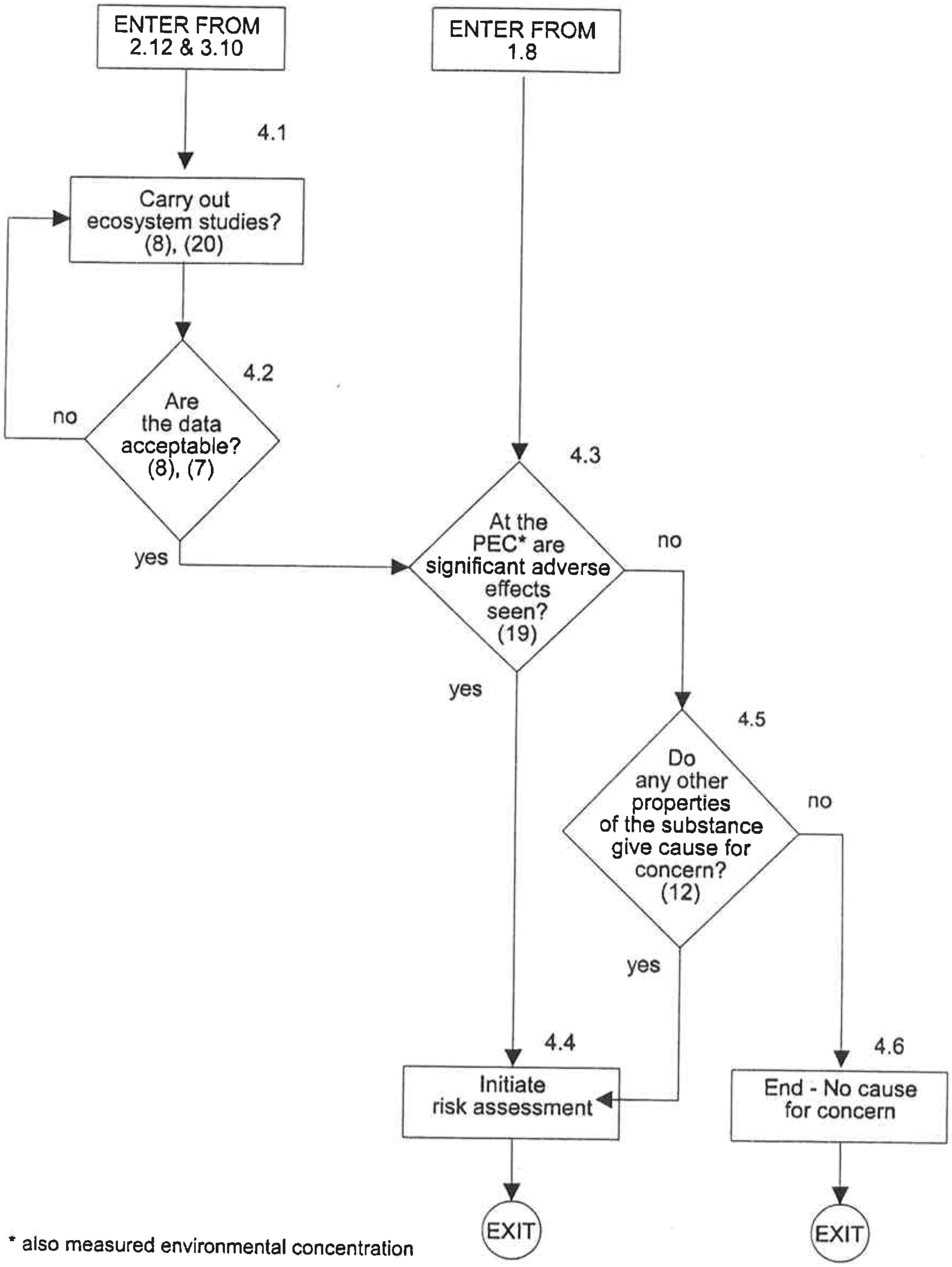
(8) For new and existing substances, studies could be carried out in model ecosystems. For existing substances the ecosystem study could be a monitoring exercise. The scale and complexity of these systems would be decided on a case by case basis.

(12) The other properties to be considered here are those related to indirect effects (Note 2).

(19) See (5). The predictive power of appropriate ecosystem studies is such that, given a NOEC, no application factor should be necessary to derive PNEC.

(20) See (8). Where the substance is to be introduced experimentally (as distinct from its existing occurrence) this should be at a concentration equivalent to a well-argued reasonable worst case, perhaps flanked by a small number of other concentrations.

FIGURE F-4
PROCESS MAPS EFFECTS ASSESSMENT, PART 4
THE USE OF ECOSYSTEM STUDIES



* also measured environmental concentration

APPENDIX G. PHYSICAL/CHEMICAL DATA OF SUBSTANCES USED IN MODEL CALCULATIONS

SUBSTANCE	BZ	LAS	DEHP	BHT	DCA	NTA
MW	78.12	347	390.57	220.34	162	191.1
melt.p (C)	5.51	10	-55	70	71.5	242.5
Vp (Pa)	11000	1×10^{-10}	7.4×10^{-5}	0.3	1.77	1×10^{-10}
Sol (mg/l)	1800	350	0.2	0.66	310	1280
Log P	2.13	2.5	4.88	4.6	2.78	1
T1/2 air (h)	134	8	24	17	6	8
T1/2 water (h)	570	35	720	240	240	72
T1/2 soil (h)	215	339	1025	133	720	240
T1/2 sed (h)	1700	17	360	120	120	20
K soil/water		1000				140
K sed/water		1000				140
K susp/water		1000				140
(BCF)						
K pr.sl. WWTP		2800				140
K sec. sl. WWTP		2800				140

MW	molecular weight
melt.p.	melting point
Vp	vapour pressure
Sol	water solubility
log P	partition coefficient octanol/water
T1/2	halflife

BCF	Bioconcentration factor
K pr.sl.WWTP	part. coeff. primary sludge in waste water treatment
K sec.sl.WWTP	part. coeff. secondary sludge in waste water treatment
Ka/b	partition coefficient medium a/medium b

APPENDIX H. PARAMETERS AND DATA USED IN PRISEC AND HAZCHEM

	PRISEC Europe	PRISEC NL	HAZ-CHEM Europe	HAZ-CHEM NL
surface area (km^2)	$4x10^6$	$4x10^4$	$4x10^6$	$4x10^4$
water surface %	4	4	4	4
industrial soil % (soil 3)	1	1	-	-
agricult.soil % ('soil 2')	15	45	15	45
natural soil % (soil 1)	80	50	81	51
height air comp (m)	1000	1000	1000	1000
depth water comp (m)	5	3	5	3
depth soil 2 (agricultral) (m)	0.05	0.05	0.1	0.1
depth soil 1 (natural) (m)	0.01	0.01	0.02	0.02
depth sediment (m)	0.03	0.03	0.15	0.15
conc suspended sediment (mg/l)	15	15	15	15
fraction organic carbon in soil	0.05	0.05	0.05	0.05
fraction organic carbon in sediment	0.05	0.05	0.05	0.05
fraction organic carbon in suspended sediment	0.05	0.05	0.05	0.05
advection residence time air (h)	7.7	0.8	184.8	19.2
advection residence time water (h)	264	62.7	6336	1504.8
advection residence time sediment (h)	$1x10^{10}$	$3x10^6$	$1.0x10^{10}$	$3x10^6$
temperature (C)	15	15	15	15
WWTP				
number of inhabitant equivalents	$2x10^8$	$1.0x10^7$	$2.0x10^8$	$1,0x10^7$
wastewater/inh/day (l/day)	150	150	150	150
conc primary sludge (g/l)	0.6	0.6	0.6	0.6
organic carbon content in primary sludge (w/w)	0.3	0.3	0.3	0.3
hydraulic retention time (h)	4	4	4	4
sludge retention time (h)	55	55	55	55
sludge conc aeration tank (g/l)	3.3	3.3	3.3	3.3
organic carbon content in secondary sludge (w/w)	0.37	0.37	0.37	0.37
biodegradation rate (1/h)	0.03	0.03	0.03	0.03
not readily biodegradable	no degradation	no degradation		

APPENDIX I. EMISSION ESTIMATIONS

	Prod. vol.	Prod. vol.	Emission	Emission		% to:		
	t/y x km^2	kg/h x km^2	t/y x km^2	kg/h x km^2	air	water	soil	WWTP
BZ	18.6	2.122	0.241065	0.0275	96.5	3	0.5	0
LAS	0.415501	0.0473992	0.415501	0.047399	0	100	0	100
DEHP	0.87453	0.0997639	0.015763	0.001798	0.05	99.95	0	0
BHT	0.0078894	0.0009	0.002564	0.000293	0	100	0	0
DCA	0.0510173	0.0058199	0.010203	0.001164	0	100	0	0
NTA	0.000416	0.0000475	0.000416	0.000047	0	100	0	100

Basis for the emission calculation:

BZ: 670,000t/y NL (36,101km^2) for all uses including gasoline, Emission = 8,700t/y (Slooff, 1988)
LAS: 15,000t/y NL (36,101km^2)
DEHP: 217,700 prod. vol. in D (248,935 km^2), Emission = 3,924t/y (BUA-Stoffbericht No. 4)
BHT: worst-case table, no data, prod. vol. (BUA-Stoffbericht No. 58)
DCA: 12,700 t/y in D (248,935 km^2) x 0.2
NTA: 1g/d/cap x 416cap/km^2

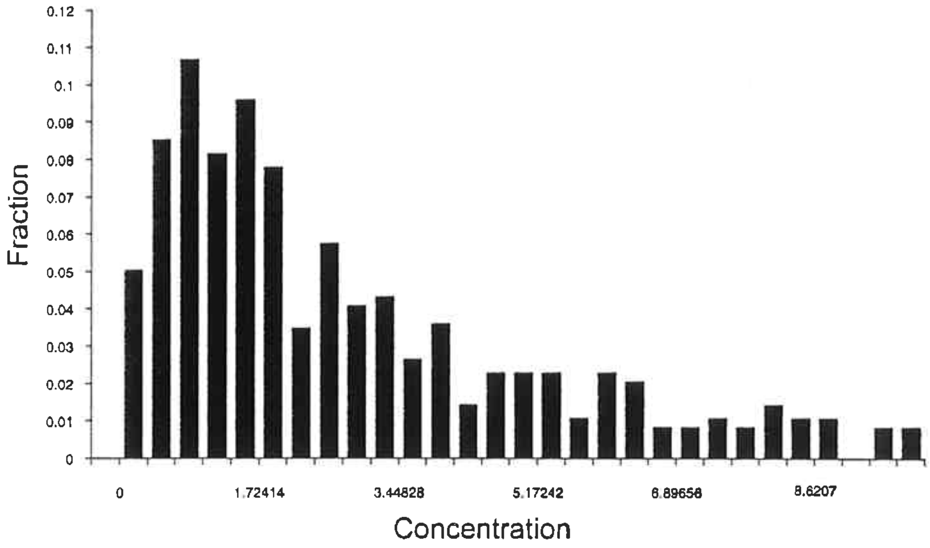
APPENDIX J. PARAMETERS FOR LAS USED IN SENSITIVITY ANALYSIS

Parameter	Distribution	Values used		
melting point [°C]	constant	10		
molecular weight	constant	347		
vapour pressure [Pascal]	constant	1.1×10^{-10}		
water solubility [mg/l]	constant	350		
log (octanol/water) p.coeff.	constant	2.5		
part. coeff. soil/water	constant	1000		
part.coeff. sediment/water	constant	1000		
part.coeff. susp.sed./water	constant	1000		
part.coeff. fish/water	constant	0		
part.coeff. prim.sludge WWTP	constant	2800		
part.coeff. sec.sludge WWTP	constant	2800		
half life in air [hours]	constant	8		
half life in water [hours]	constant	35		
half life in soil [hours]	constant	339		
half life in sediment [hours]	constant	17		
tolerable daily int. [mg/kg]	constant	0.1		
no effect.conc.aquat. [mg/l]	constant	0.1		
production volume [kg/hour]	constant	1896		
fract.of production closed	constant	0		
closed emission to air	constant	0		
closed emission to water	constant	1		
closed emission to soil	constant	0		
fract.of production matrix	constant	0		
matrix emission to air	constant	0		
matrix emission to water	constant	1		
matrix emission to soil	constant	0		
fract.of production non-disp.	constant	0		
non-disp. emission to air	constant	0		
non-disp. emission to water	constant	1		
non-disp. emission to soil	constant	0		
fract.of production disp.	constant	1		
disp. emission to air	constant	0		
disp. emission to water	constant	1		
disp. emission to soil	constant	0		
fr.water discharge to WWTP	lognormal	0.8	0.6	0.95
total surface area	constant	40000		
water surface fraction	lognormal	0.04	0.008	0.2
arable land fraction	lognormal	0.45	0.23	0.9
height aircompartment [m]	lognormal	500	200	2000
depth watercompartment [m]	lognormal	3	0.5	10
depth arable soilcpmt. [m]	lognormal	0.05	0.02	0.5
depth natural soilcpmt. [m]	lognormal	0.02	0.01	0.04
depth sedimentcpmt. [m]	lognormal	0.03	0.003	0.3
conc.susp.sed.in water [mg/l]	lognormal	15	3	75
fraction org.carbon soil	lognormal	0.05	0.01	0.25
fraction org. carbon sediment	lognormal	0.1	0.0125	0.8
fraction org.carbon susp.sed	lognormal	0.2	0.08	0.5
advect.resid. time air [h]	lognormal	60	12	300
advect.resid. time water [h]	lognormal	1440	450	4600
advect.resid. time sed [h]	lognormal	20000	4000	100000
temperature of system [°C]	lognormal	15	7.5	30
number of inhabitant equival	constant	1×10^{7}		
waste water/inhabit. [l/day]	lognormal	150	75	300
concentr.prim.sludge [g/l]	lognormal	0.6	0.4	0.9
O.C.-content prim.sludge w/w	lognormal	0.3	0.25	0.36
hydraulic retention time [h]	lognormal	12	4	36
sludge retention time [h]	constant	0		
sludge conc.aerat.tank [g/l]	lognormal	4	2	6
O.C.-content sec.sludge w/w	lognormal	0.4	0.33	0.48
biodegrad.rate BODtest [l/h]	lognormal	0.03	0.02	0.045

APPENDIX K. SENSITIVITY ANALYSIS, CONCENTRATIONS OF LAS IN SUSPENDED MATTER AND IN WATER.

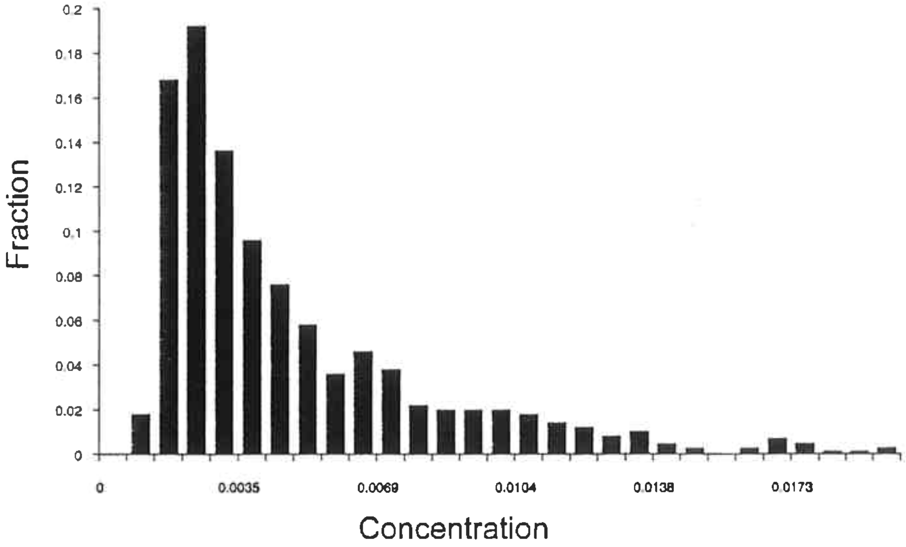
SUSPENDED MATTER CONCENTRATION (PPM)

each column is 0.344828 wide



DISSOLVED WATER CONCENTRATION (mg/l)

each column is 0.00069 wide



APPENDIX L. LOCAL MODEL FOR THE AQUATIC COMPARTMENT

Substance	NTA						LAS					
Substance notified/marketed/used (kg/cap x yr)	0.37						1.66					
Water consumptionm (l/capita x day)	200						200					
assumed dilution factor	10						10					
	Screening		Confirmatory		Investigative		Screening		Confirmatory		Investigative	
	% removal	% biodeg.	% removal	% biodeg.	% removal	% biodeg.	% removal	% biodeg.	% removal	% biodeg.	% removal	% biodeg.
Fate of Substance During Treatment												
Primary treatment % removal	1.3	0	1.9	0	20	NA	10.8	0	26.1	0	35	NA
Primary + secondary treatment % removal	67.0	58.0	90.1	84.7	95	NA	94.8	73	98.6	67	99	NA
Primary + secondary + tertiary treatment % removal	67.0	58.0	90.1	84.7	95	NA	94.8	73	98.6	67	99	NA
PEC (µg/l) sewage effluent												
Raw sewage	5002		5002		6849		22747		22747		22747	
Prim. treatment effluent	4937		4907		5479		20291		16810		14786	
Prim. + sec. treatment effluent	1651		495		342		1183		318		227	
Prim. + sec. + tert. treatment effluent	1651		495		342		1183		318		227	
PEC (µg/l) River Water												
below UNTREATED outfall	500		500		685		2275		2275			
below primary treatment outfall	494		491		548		2029		1681		1479	
below prim. + second. treatment outfall	165		50		34		118		32		23	
below prim. + second. + tert. treatment outfall	165		50		34		118		32		23	
PEC (mg/kg) sludge wastage												
primary before anaerobic treatment	24		35		NA		909		2197		NA	
secondary before anaerobic treatment	86		51		NA		942		1366		NA	
Population (millions)	25						25					
Incidence of sewage treatment facilities												
Untreated	12						12					
Primary	10						10					
Primary + secondary	70						70					
Primary + secondary + tertiary	8						8					

APPENDIX M. PGTREAT: WWTP MODEL.

PART 1: INPUT DATA

	Screening	Confirmatory	Screening	Confirmatory
Substance	LAS		NTA	
MW	348	348	200	220
SOL (mg/l)	350	350	500	500
VP (mm)	$7.60x10^{-11}$	$7.60x10^{-11}$	$7.60x10^{-11}$	$7.60x10^{-11}$
LOG P	3		2	
LOG Kd	3	3.54		2.17
H (atm x m^3/mol)	$9.94x10^{-14}$	$9.94x10^{-14}$	$4.0x10^{-14}$	$4.4x10^{-14}$
k (d-1)	0.7	0.85	0.7	2.4

PART 2: PREDICTIONS

	Screening	Confirmatory	Screening	Confirmatory
Substance	LAS		NTA	
Total removal rate (%):	94.8	98.6	67.0	90.1
Total primary removal (%)	10.8	26.1	1.3	1.9
Percent substance adsorbed	71.4	89.7	20.0	27.0
Percent removal by sorption	21.7	34.1	9.0	5.3
Percent removal by volatilization	0.0	0.0	0.0	0.0
Percent removal by biodegradation	73.1	64.5	58.0	84.7
Output data				
Chemical Consumption (g/cap.day)	4.55	4.55	365.12	1.00
Water Consumption (l/cap.day)	200	200	200	200
Influent chemical conc (µg/l):	22747.20	22747.20	1825584.00	5001.60
Primary Treatment Module				
Influent chemical conc (µg/l):	22747.20	22747.20	1825584.00	5001.60
Influent susp solids (mg/l):	220.0	220.0	220.0	220.0
Suspended solid removal(%):	60.0	60.0	60.0	60.0
Partition coeff (l/kg):	1000.0	3500.0	100.0	148.0
Conc. on prim. sludge (µg/l):	4101.95	9895.67	39298.29	157.72
Effluent susp solids (mg/l):	88.0	88.0	88.0	88.0
Tot. Effl. chem. conc. (µg/l)	20286.0	16809.8	1802005.0	4907.0
Dissolved Effl. conc. (µg/l)	18645.2	12851.5	1786285.7	4843.9
Sorbed Effl. conc. (µg/l)	1640.8	3958.3	15719.3	
Tot. Prim. removal (%):	**10.82**	**26.10**	**1.29**	**1.89**
Activated Sludge Module				
Influent chemical conc (µg/l):	20286.03	16809.80	1802005.03	4906.97
[Q],Wastewater flowrate (m^3)	155.0	155.0	155.0	155.0
[G],Airflow(m3air):Q (m^3water):	5.4	5.4	5.4	5.4
[Rh], Hyd residence time (d):	0.290	0.290	0.290	0.290
[Rs], Sludge retention time:	9	9	9	9
[H], Henrys Law (atm-m^3/mole):	9.94×10^{-14}	9.94×10^{-14}	4.00×10^{-14}	4.40×10^{-14}
[R], Gas const(m^3-atm/K-mole):	0.000082	0.000082	0.000082	0.000082
[Kp], Partition coeff (l/kg):	1000.0	3500.0	100.0	148.0
[X], MLSS (mg/l):	2500.0	2500.0	2500.0	2500.0
ka: sludge biod. (d-1)	0.7	0.85	0.7	2.4
kb: aqueous biodeg. (d-1)	0.7	0.85	0.7	2.4
[k1],biodeg. term:	4.56	6.89	1.42	6.34
[T], Temperature (K):	293.0	293.0	293.0	293.0
Sludge removal fraction:	0.95	0.95	0.95	0.95
Reactor concentration (µg/l):	3649.88	2130.34	743892.43	668.38
Liquid Effluent conc. (µg/l):	1173.18	314.09	602552.87	496.89
Sludge conc. (µg/l)	2607.06	1911.84	148778.49	180.51
Activated Sludge removal (%):	**94.22**	**98.13**	**66.56**	**89.87**
Conc. on ASM sludge (µg/l)	2607.06	1911.84	148778.49	180.51
Conc. ASM sludge (mg/kg)	1042.82	764.74	59511.39	72.20
Conc. on prim. sludge (mg/kg)	18645.25	44980.34	178628.57	716.89
Total conc. on sludge (mg/kg)	11604.28	27294.10	130981.70	459.02

APPENDIX N. EXAMPLE OF A GENERIC EXPOSURE SCENARIO FOR A TEXTILE DYE

GENERAL LOCAL PROCEDURE	CALCULATION EXAMPLE
Use pattern	textile dye
purity	81.5 %
consumption during use	specific dye consumption: 2-5kg dye/t fibre with fixation degree: 98-99 %
waste water production	specific waste water production: 50m^3/t fibre
dye concentration in process waste water	0.02-0.1kg/t fibre non fixed dye = 0.3-1.6g/m^3
internal dilution	waste water of the plant: 100m^3/h, lot size: 0.6t, colouring time: 3h dilution factor = 10
dilution in the sewage treatment plant	dilution factor in the sewage treatment plant (1000m^3/h) = 10
dilution during release of the waste water treatment plant into e.g. a river	dilution factor for outlet into river (50,000m^3/h) = 50
total dilution factor: process waste water -> river	10 x 10 x 50 = 5000
initial PEC without elimination	PEC = 0.06-0.32mg/m^3
Removal during waste water treatment (e.g. sorption)	Removal = 60-90%
elimination factor	2.5-10 (worst case: 2.5)
generic environmental concentration	PEC_{river} = 0.02-0.12mg/m^3

APPENDIX O. RESULT OF HAZARD ASSESSMENT FOR THE AQUATIC COMPARTMENT ON NTA & BHT

PEC/PNEC ratios

Environmental Compartment: Water
Substance: NTA

EFFECT / EXPOSURE	ACUTE		CHRONIC		ECOSYSTEM	
LEVEL / PHASE	Regional	Local	Regional	Local	Regional	Local
SCREENING	1.9×10^{-6}	0.2	$\boxed{2.9\times10^{-7}}$	0.03		
CONFIRMATORY		0.06		0.01		
INVESTIGATIVE		0.04		$\boxed{0.006}$		

	ONGOING	FINAL
Status of Hazard Assessment		X

☐ Most reliable PEC/PNEC ▨ Next Step

PEC/PNEC ratios

Environmental Compartment: Water
Substance: BHT

EFFECT / EXPOSURE	ACUTE		CHRONIC		ECOSYSTEM	
LEVEL / PHASE	Regional	Local	Regional	Local	Regional	Local
SCREENING	0.0005		$\boxed{0.0013}$	▨		
CONFIRMATORY						
INVESTIGATIVE						

	ONGOING	FINAL
Status of Hazard Assessment	X	

☐ Most reliable PEC/PNEC ▨ Next Step

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