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RIVM GUIDANCE DOCUMENT

Ecotoxicological Effect Assessment: Deriving Maximum Tolerable Concentrations (MTC) from single-species toxicity data

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CONTENT

SUMMARY

In the last few years there has been a rapid development in methodologies to determine environmental concentrations of chemical substances at which adverse effects on ecosystems are not likely to occur. In the international upswing of the ecotoxicological effect assessment The Netherlands plays an important role. The Dutch publication wave, however, threatens to result in a continuously updating of evaluation methods, disabling consistent standard setting procedures. Therefore this report ties down the method of ecotoxicological effect assessment at a level that is currently accepted in The Netherlands and is to be used as a guidance document in the advisory work of the RIVM for the next few years.

The document describes an initial and a more refined method to extrapolate from single-species toxicity data to maximum tolerable concentrations (MTCs) of chemical substances in water, sediment, soil, groundwater and air. Starting point is that the maximum tolerable concentration is set equal to the best estimate of the concentration at which the no-observed-effect-level of 95% of the species in an ecosystem is not exceeded. Checks are included to prevent top predators from secondary poisoning and ecological functioning from detoriation by harming microbiological processes. In case the data base is limited a more conservative approach is used, applying assessment factors to the available toxicity data.

It is recognized that there are various factors that are not included in the outlined procedure and several aspects need further discussion. Therefore this report also presents recommendations for future research and decision-making activities.

Keywords: ecotoxicology, effect assessment, extrapolation, maximum tolerable concentrations

1. INTRODUCTION

The concept of risk assessment, currently being used in The Netherlands, was first introduced in the 1986-1990 Multi-year Programme for Environmental Management. Coming to terms with environmental risks of chemical compounds is not only a scientific matter. Although risks can be quantified scientifically, standards are set by politicians. Recently it was decided to distinguish a maximum tolerable level and a negligible level (VROM, 1989). As to ecosystems it was decided that a chemical should not affect populations of more than 5% of the species. Hence, the maximum tolerable level is chosen as that environmental concentration of a compound at which (theoretically) 95% of the species in an ecosystem is fully protected. The negligible level is chosen as 1% of the MTC or, in case of natural compounds, as the concentration measured in relatively unpolluted areas ("background" concentrations).

There is no scientific basis for setting the maximum tolerable concentration at a 95% protection level, nor are there scientifically sound arguments to consider 1% of this level to have a negligible effect for the structure and functioning of ecosystems. However, the acceptability of these concentration levels are the result of continuous interaction between policy makers and scientists. Before coming to a risk philosophy much attention has been paid by the scientific community to estimate concentrations in environmental compartments, that are "safe" to ecosystems. The rapid development of extrapolation procedures used to derive acceptable concentrations of chemicals in the environment has led to several adaptations of the effect assessment procedure used in advisory reports of the National Institute of Public Health and Environmental Protection (RIVM) published in recent years. Also throughout the years different criteria have been used in determining the reliability of (literature) toxicity data and in assessing the experimental no-observed-effect concentrations. As a result the recommended maximum tolerable concentration for a given compound may have been changed in the past few years and the reasons why have not always been clear. To avoid further confusion and to standardize advisory work by the RIVM it was decided to tie down the handling of ecotoxicological literature data in advisory work in terms of recommending maximum tolerable levels, as done in the present report.

It should be noted that the following aspects are not dealt with in this report:

[a] criteria for determining the reliability of literature data,

[b] factors that may play a role in determining standards for each environmental compartment (such as background concentrations, combined toxicity, persistence and the possible role of the substances as micro nutrients),

[c] coordination of the maximum tolerable concentrations of the different environmental compartments.

The present report is meant as a guidance document for those who are involved in advisory work for environmental policy makers and will be used as a basis for ecotoxicological effect assessment by the RIVM. The procedure presented should be applied for some years without radical changes. Therefore those parts that are still in discussion have been left out. In fact, while drawing up this report it became evident that still much needs further research and discussion and several procedures may be reconsidered when sufficient support becomes available. Hence, apart from being a guidance document presenting the current methodology of deriving MTCs from single-species toxicity data, the report also includes discussions and recommendations for future activities (Multi-year Activity Program 1993).

It is stressed that the methods presented should be considered as a basis for ecotoxicological effect assessment; deviations may be possible provided they are underpinned by sound arguments.

2. HISTORICAL BACKGROUND

2.1. National activities

In this section the historical development of the ecotoxicological effect assessment of chemicals is briefly outlined, focussing on the procedures used in the Netherlands.

In 1979 Canton and Slooff proposed to consider the lowest NOEC (or NOLC) multiplied by the quotient of the EC25 (or LC25) and the EC50 (or LC50) (based on long-term toxicity tests with different freshwater organisms) as water quality criterion. At that time there was little discussion about extrapolating toxicity data to "safe" concentrations and the method has never been used or adopted as such.

Several years later Slooff et al. (1986) performed linear regression analyses between data sets on acute, chronic and (semi)field aquatic toxicity. The equations were used to predict chronic toxicity on the basis of acute toxicity data and to predict "safe" concentrations for aquatic ecosystems on the basis of single species acute or chronic data. This method has been used in the eighties in the effect assessment of both new and existing chemicals.

Kooijman (1987) assumed the distribution of the log of the sensitivities of species to a toxicant to be logistic. He showed the validity of this assumption based on laboratory data from Slooff et al. (1983). According to this approach each species tested represents an estimate of the sensitivity of a biotic part of the ecosystem. Based on several of such estimates, the range of sensitivities for all species can be approximated. The main advantage is that this method provides a unifying ecotoxicological concept. Although not intended by the author (calculating a hazardous concentration based on LC50 values), the method as such was used for calculating "safe" concentrations. In fact the procedure is the very basic model to extrapolate the effects at the species level to the effect at the level of the ecosystem and meets the requirements for estimating risks.

Van Straalen and Denneman (1989) modified the procedure of Kooijman (1987) and originally applied the method for effect assessment in terrestrial environments. Because of its general concept the method is applicable to each environmental compartment providing analogous assumptions are used. The modifications were found to be improvements. The major modifications were (a) the use of chronic NOEC-values instead of LC50s, (b) the independency of species number in hypothetical ecosystems and (c) the possibility to choose different protection concentrations (e.g. 95% of all species).

Since a situation has been developed that different methods were applied simultaneously to estimate ecotoxicologically maximum tolerable concentrations in environmental compartments, The Netherlands Health Council (1989) was requested by the government to evaluate the ecotoxicological extrapolation methods. From an inventory it appeared that, apart from the above-mentioned Dutch methods, only proposals from the United States were available (EPA, 1984; Blanck, 1984; Stephan et al., 1985). Based on the information available the Health Council recommended to use all three Dutch proposals (Slooff et al., 1986; Kooijman, 1987; Van Straalen and Denneman, 1989) for effect assessment, each with its specific function, applying the method of Van Straalen en Denneman as a basis (using the 95% protection concentration level). The Council also recommended to use at least three chronic NOEC values determined for species different in ecological function, anatomic design and different routes of exposure.

At about the same time DBW/RIZA (1989) published a procedure to derive a basic quality level in water offering opportunities for life for aquatic communities including higher organisms and also protecting ecological interests outside the water (fish-eating birds and mammals). In this method the lowest NOEC-value determined for an alga, mollusc, crustacean and fish is considered to provide sufficient protection for aquatic ecosystems. For several compounds (such as PCBs, PAHs and metals) correction factors are applied to account for combined effects of chemicals with similar modes of action. With respect to poisoning along the food chain, the concentration standards in products (standards for protecting human health) are converted to water quality requirements. This procedure was adopted in the Third Water Action Program.

In the same year the Directorate General for the Environment of the Dutch Ministry for Housing, Physical Planning and Environment published risk limits in the context of environmental policy, adopting the 95% protection concentration as the basis for deriving the maximum tolerable concentration (VROM, 1989). The Directorate General for the Environment initiated a study by the RIVM in order to derive a coordinated set of environmental quality standards for water and soil based on this risk philosophy. In this study (Van de Meent et al., 1990) the advice of the National Health Council was used as a basis. However, several modifications were made:

- The statistical procedure of Van Straalen and Denneman (1989) did not achieve its nominal confidence level for the lower limit of the 95% protection level. Therefore other statistics were used (Bayesian statistics instead of sampling statistics).
- At least four chronic NOEC values for different taxonomical groups were required to reduce the uncertainty in the estimate of the maximum tolerable concentration (Okkerman et al., 1992).
- NOEC values of taxonomically related species were grouped at the level of classes to get a more representative sample of species in an ecosystem (which is not to be confused with a random sample, as required by the method of Kooijman and modifications thereof).
- In case insufficient data were available to derive a maximum tolerable concentration it was proposed to use a simple system based on the EPA (1984) to make an indicative judgement of the effect of a compound, applying an assessment factor of 10 to 1,000, depending on the toxicological data available.

In 1991 the study of Van de Meent et al. (1990) was extended paying attention to secondary poisoning. Instead of converting product standards to environmental quality requirements as performed by DBW/RIZA (1989) a general algorithm was proposed to include critical biomagnification pathways in aquatic and terrestric ecosystems (Romijn, 1991a,b; Jonkers and Everts, 1991).

More recently Aldenberg and Slob (1992) improved the modification of the Van Straalen and Denneman method to account for the uncertainty in the 95% protection level estimate and discussed the theoretical risk of protecting substantially less than 95% of the biological species.

2.2. International activities

Also at the international level the assessment of exposure, effect and risk is in discussion. In the last year several special workshops were hold, a.o.:

- In September 1990 an OECD workshop on the Application of QSARs to Estimate Toxicity Data was held in Utrecht (The Netherlands). Also the 4th International Workshop on QSAR in Environmental Toxicology was held in September 1990 in Veldhoven (The Netherlands), indicating a world-wide increase of research efforts in this field (Hermans and Opperhuizen, 1991).
- In December 1990 an OECD workshop on Aquatic Effect Assessment was held in the USA. Aldenberg and Slob (1991) presented an improved procedure based on the original sampling statistics used by Van Straalen and Denneman (1989). Similar methods were developed by the EPA (assuming a.o. a triangular distribution of species sensitivities; Stephan et al., 1985) and by Wagner and Lokke (1990; assuming a log-normal distribution of species sensitivities). At this workshop one agreed upon the use of a modification of the EPA (1984) procedure, in case the data are insufficient to apply statistical extrapolation methods.
- In May 1991 an OECD workshop on Effect Assessment of Chemicals in Sediment was held in Copenhagen (Denmark). Various methods were recommended to derive quality standars for chemicals in sediments.
- In June 1991 an US-Dutch workshop was held on Comparative Risk Analysis Approaches for Air Pollution Prevention (Seattle, USA). At this workshop The Netherlands proposed to follow basically the same procedure for effect assessment for air pollutants as was agreed upon for water pollutants at the December OECD workshop.

3. ECOTOXICOLOGICAL DERIVATION OF MAXIMUM TOLERABLE LEVELS

3.1. General approach

A MTC of a chemical substance in the environment is the maximum concentration of that chemical at which unacceptable adverse effects on the ecosystem are not likely to occur. A definition of "unacceptable" is of political concern and has been presented in the policy document "Premises for Risk Management".
Since ecosystems are compartimentalized into soil and groundwater, surfacewater and sediments (freshwater and marine) and air, a methodology is presented to determine maximum concentrations of chemical substances in each of these environmental compartments based on observed or expected effects in representative species inhabiting these compartments or in species that predate on these species (secondary poisoning).

The approach to estimate a maximum tolerable concentration depends on the information available. In this respect the OECD (1991) distinguished a comprehensive, refined and a preliminary effect assessment, with decreasing amount of information.
Ideally, the effects of a substance should be tested in a natural system representative of the area to be protected, the results to be used in a comprehensive effect assessment. However, isomorphic testing is scarce and the (few) studies in various complex systems (including multi-species laboratory systems, microcosms, and field trials) are hard to evaluate (Okkerman et al., 1992; Emans et al., 1992). Therefore in this document the derivation of maximum tolerable concentrations from information on physico-chemical characteristics and single-species toxicity is presented only.

When chronic toxicity data on a substance for 4 or more species of different taxonomic groups are available for a particular environmental compartment, a procedure is applied to extrapolate from the available single-species toxicity data to all species in that ecosystem compartment (refined effect assessment, see chapter 4).

If less information is available on the ecotoxicity of the compound a set of assessment factors are applied, varying from 10 to 1,000 dependant on the available information (preliminary effect assessment, see chapter 5).

If no toxicity data on species representative for an ecosystem compartment are available, the maximum tolerable concentration of a substance may be derived from that determined for other environmental compartments based on the concept of equilibrium partitioning. Hence, the maximum tolerable concentration of a substance in sediment, soil and air may be derived from the maximum tolerable concentration of that substance in water by applying partition coefficients: Kp sediment-water, Kp soil-water and Kh air-water respectively (see 3.2b and 5).

It should be realised that there is a distinct difference in the information available on the toxicity of substances between the various environmental compartments. Most information is available on the aquatic environment. This is not the case for the soil compartment: soil toxicity data are scarce and most tests are still in development. However, the information on soil toxicity of substances is growing fast. Even less developed is the knowledge of the effects of chemical compounds to which species are exposed through groundwater and air. In spite of these differences in knowledge methods for soil, groundwater and air effect assessment are proposed following a similar basic approach in striving towards a consistent methodology.

3.2. Literature search, data handling, effect assessment

In order to derive proposals for maximum tolerable levels of chemicals three stages can be distinguished:

a] Literature search and determination of reliable data

In this report no attention is given to this stage. Information on literature search and selection criteria involved in determining the reliability of data will be published separately in spring 1992.

b] <u>Handling of the literature data to obtain reliable input data for effect assessment model calculations</u>

Toxicity data

Only those toxicological criteria are taken into account that exclusively may affect the species on the level of population. Primarily these are survival, growth and reproduction (including [histopathological] effects on reproductive organs, spermatogenesis, fertility, pregnancy rate, number of eggs produced, egg fertility, eggshell thickness, hatchability etc.) (**see chapter 6, point 1**).

Data should be expressed as L(E)C50 (short-term tests, duration 4 days or less) or NOL(E)C (long-term tests, duration more than 4 days, with the exception of micro-organisms for which an NOL(E)C-value may be derived from experiments during less than 4 days). For birds the LC50 test usually takes 5 days of exposure. The NOEC is the highest concentration/dose tested in a series of test concentrations causing no significant effect (**see chapter 6, point 2**).

Regarding toxicity data handling the following rules are used:

- If for one test species several toxicity data based on the same toxicological endpoint are available, these values are averaged by calculating the geometric mean (**see chapter 6, point 3**).
- If for one test species several toxicity data are available based on different toxicological endpoints, only the lowest value is used.
- Toxicity data will not be clustered according to taxonomic group (**see chapter 6, point 4**).
- Freshwater and marine toxicity data are combined unless analysis of the data indicates otherwise (e.g. because of difference in bioavailability of the compound).

Data on partition coefficients

In case no toxicity data on species inhabiting an environmental compartment are not available, partition coefficients are used to derive MTCs from those determined for other ecosystem compartments. For example, the MTCs for sediment and soil may be derived from the MTC determined for surfacewater using the partition coefficient K_p, whereas the MTC for air may be derived from the MTC for surfacewater using the Henry coefficient K_h.

Partition coefficient water/sediment and water/soil

To estimate the K_p and BCF (see below) of organic compounds a similar approach is followed:

- The K_p is preferably determined as the geometric mean of representative experimental data.
- In case no experimental data are available or the representativeness is doubted (e.g. in case it is expected that the exposure time is insufficient to reach a steady-state) the K_p is calculated using the formula

  $K_p = K_{oc} * f_{oc}$ and $K_{oc} = K_{ow}$, where

  K_{oc} = organic carbon referenced partition coefficient [l water.kg^{-1} organic carbon]

  f_{oc} = fraction organic carbon in sediment or soil [kg organic carbon.kg^{-1} dry sediment or soil], fixed at 5%

This leads to the formula: $K_p = 0.05 . K_{ow}$

- Acidic organic compounds may dissociate and the ions are far less hydrophobic than their uncharged equivalents. The fraction of the non-dissociated substance (f_{ni}) is calculated from the dissociation constant pK_a and the pH. For these chemicals (a.o. phenolic compounds) the following model accounting for the degree of ionization is used:

  $K_p = f_{oc} * K_{ow} * f_{ni}$, where $f_{ni} = 1/(1 + 10^{pH-pKa})$.

  The pH is fixed at 6 (soil) or 8 (sediment)(***see chapter 6, point 5***).

For inorganic compounds (heavy metals) K_p -values can only be derived from literature data, since no general partition model is available. Practice learns that the K_p-values in the field show a great variability and depend on many confounding factors e.g. pH, salinity, dissolved oxygen. For example the mean K_p-values for metals in large water bodies in The Netherlands vary a factor of 5-10, the individual measurements showing a much greater variation (Van der Kooij et al., 1991).

Hence, the use of the K_p is only valid when applied to the environment for which the K_p was measured. An indication of K_p-values for heavy metals in large water bodies in The Netherlands is given in table 1.

Table 1 *K_p-values (in l/g, mean values over the period 1983-1986) for Dutch surface waters (after Van der Kooij et al., 1991), extreme values underlined*

Water body	*Cr*	*Cu*	*Hg*	*Cd*	*Zn*	*Ni*	*Pb*	*As*
Rhine (Lobith)	*200*	*32*	*120*	*82*	*81*	*8.3*	*520*	*11*
Rhine (Hagenstein)	*310*	*45*	*270*	*170*	*110*	*7.3*	*560*	*18*
Waal	*230*	*36*	*180*	*140*	*100*	*7.7*	*630*	*9.0*
Meuse (Eijsden)	*160*	*56*	*190*	*360*	*220*	*11*	*690*	*10*
Haringvliet	*786*	*55*	*125*	*63*	*190*	*22*	*440*	*7.8*
West Scheldt O	*320*	*67*	*170*	*77*	*58*	*4.3*	*860*	*7.6*
West Scheldt W	*230*	*12*	*31*		*57*	*11*	*640*	*10*
Lake Ketel	*300*	*50*	*250*	*150*	*140*	*9.1*	*690*	*5.4*
Lake IJssel	*130*	*48*	*73*	*65*	*220*	*12*	*500*	*7.0*
Nieuwe Merwede	*280*	*40*	*134*	*120*	*120*	*6.2*	*870*	*18*
Nieuwe Waterweg	*320*	*47*	*210*	*50*	*81*	*7.5*	*580*	*11*
Old Meuse	*270*	*45*	*210*	*160*	*170*	*7.5*	*1000*	*8.5*
Kan.Gent/Tern.	*310*	*150*	*180*	*490*	*52*	*5.6*	*3500*	*17*
Median	*290*	*50*	*170*	*130*	*110*	*8*	*640*	*10*

Although it is well known that metals can form insoluble sulfides, it has been recognized only recently that that acid volatile sulfide (AVS) is a reactive pool of solid phase sulfide that is available to bind with metals. This information may be used in determining maximum tolerable concentrationsw of heavy metals (see 5.3).

Partition coefficient for water/air

If information on the Henry coefficient is not available, the Henry coefficient may be estimated by dividing the vapour pressure by the water solubility of the compound according to the environmental characteristics of the Netherlands as described in SimpleRisk (Van de Meent, 1989). In case no quantitative data on the water solubility (S_w) are available, the S_w can be estimated from the following equations:

For liquid compounds: $\log S_w = -1.16 \log K_{ow} + 0.70$

For solid compounds: $\log S_w = -1.16 \log K_{ow} - 0.009 (T_m - 25)$

in which: S_w : water solubility

T_m : melting point

In case the melting point is not available the following equation can be used:

$$\log S_w = -1.23 \log K_{ow} + 0.79$$

Data on bioconcentration factors (BCF)

The BCF (bioconcentration factor) is defined as the concentration in a species at steady state divided by the mean concentration of the substance in the species' environment during exposure period. For some chemicals the BCF may be estimated from the characteristics of the chemical (octanol-water partition coeffient: K_{ow}).

Considering bioaccumulation data the following rules are taken into account for the freshwater and marine water:

- The BCF in the food (fish and mussels) is preferably determined as the geometric mean of experimental data (first to be determined within one species, subsequently determined as the geometric mean for all species). BCFs determined for fish and mussels are combined unless the data indicate that the BCFs for fish and mussels are different. The reason to prefer experimentally derived BCFs is that other processes may influence bioaccumulation which are included in the experimental results (e.g. metabolization).
- To indicate a worst case also the highest BCF is used.
- In case no experimental data are available, the method to be followed depends on the chemical and the environmental compartment

For inorganic, organo-metallic, instable, volatile, ionogenic or dissociating compounds and organic compounds with a log $K_{ow} > 6$ or a molecular weight > 600 g the geometric mean of reliable field data is used.
For the remaining (neutral) organic chemicals the BCF is derived using the formula BCF = 0.05 K_{ow} (MacKay, 1982) for the aquatic environment (based on an average of 5% lipid content in fish).

For terrestrial ecosystems the situation is much more complicated and the procedure to be followed is not accepted widely.

- Bioconcentration soil - plant
  The uptake by plants is determined by the availability in the pore water, the uptake by the roots and the transportation from root to other parts of the plant. Pore water concentrations are determined by applying the partition coefficient. The concentration in the plant is calculated as:

  $C_{pl} = C_{pw} \times TSCF \times SCF$ (Briggs et al., 1982, 1983)
  in which:
  C_{pl} = concentration in the plant (mg/kg wwt)
  C_{pw} = concentration in the pore water (mg/l)
  TSCF = transportation stream concentration factor:
  $0.75 \cdot \exp[-\log(K_{ow}) - 1.76)^2 / 2.44]$ ((mg/l)/(mg/l)
  SCF = transportation stream concentration factor, in which:
  $\log(SCF-0.82) = 0.95 \log K_{ow} - 2$ (l/kg)

- Bioconcentration soil - soil and litter organisms
  For soil organisms the BCF of organic compounds may be considered constant, dependent on the lipid content of the prey and the organic carbon content of the soil (Romijn et al., 1991b). The organic carbon content is rounded and fixed at 5% (according to the calculation [% organic matter (10) = % organic carbon x 1.7] this is about 6%). For earthworms the lipid content is set at 1% (varying from 0.5-2.5% on fresh weight basis as determined for various species: E. andrei, E. fetida and A. caliginosa; Lee, 1985; Belfroid et al., in press), resulting in a BCF of 0.4. For springtails and isopods these levels are about 1-4% (pers. comm. VU, Amsterdam, 1992), corresponding to the

levels quoted for soil organisms in general (Swift et al., 1979). Therefore for the general algorithm the lipid level is fixed at 2.5% for soil organisms, resulting in a BCF-value of 1 as a mean value. For a worst case approach a BCF of 10 is used.

- Bioconcentration, others (**see chapter 6, point 6**)

For heavy metals specific QSARs may be available to follow the refined assessment procedure (for example cadmium, see Ma, 1982).

c] Running the effect assessment model calculations

As stated above, in the effect assessment based on single-species toxicity data a distinction is made between a preliminary effect assessment procedure and a refined effect assessment procedure, the use being dependent on the nature and amount of available information.
Preferably the refined procedure is to be followed to estimate a MTC of a substance. In this procedure the sensitivity to a compound as experimentally determined for a few species is extrapolated to the whole community of species. The minimum information required to run this model is the availability of four chronic NOEC-values for different species. This method is outlined in chapter 4.
The preliminary effect assessment procedure will be applied only in case insufficient data are available. In this procedure data are not extrapolated but simple assessment factors are applied. Information is considered insufficient in case less than four chronic NOEC-values for different species are available. This method is described in chapter 5.

Usually the values obtained with the preliminary procedure will be more conservative than those obtained with the refined procedure (Van de Meent et al., 1990; Romijn et al., 1992). This is desirable since judgemental prudence dictates that substantial assessment factors be employed when only a few data are available.

In figure 1 the approach in the ecotoxicological effect assessment is schematically presented to provide guidance for deriving maximum tolerable concentrations from single-species toxicity data for each ecosystem compartment.

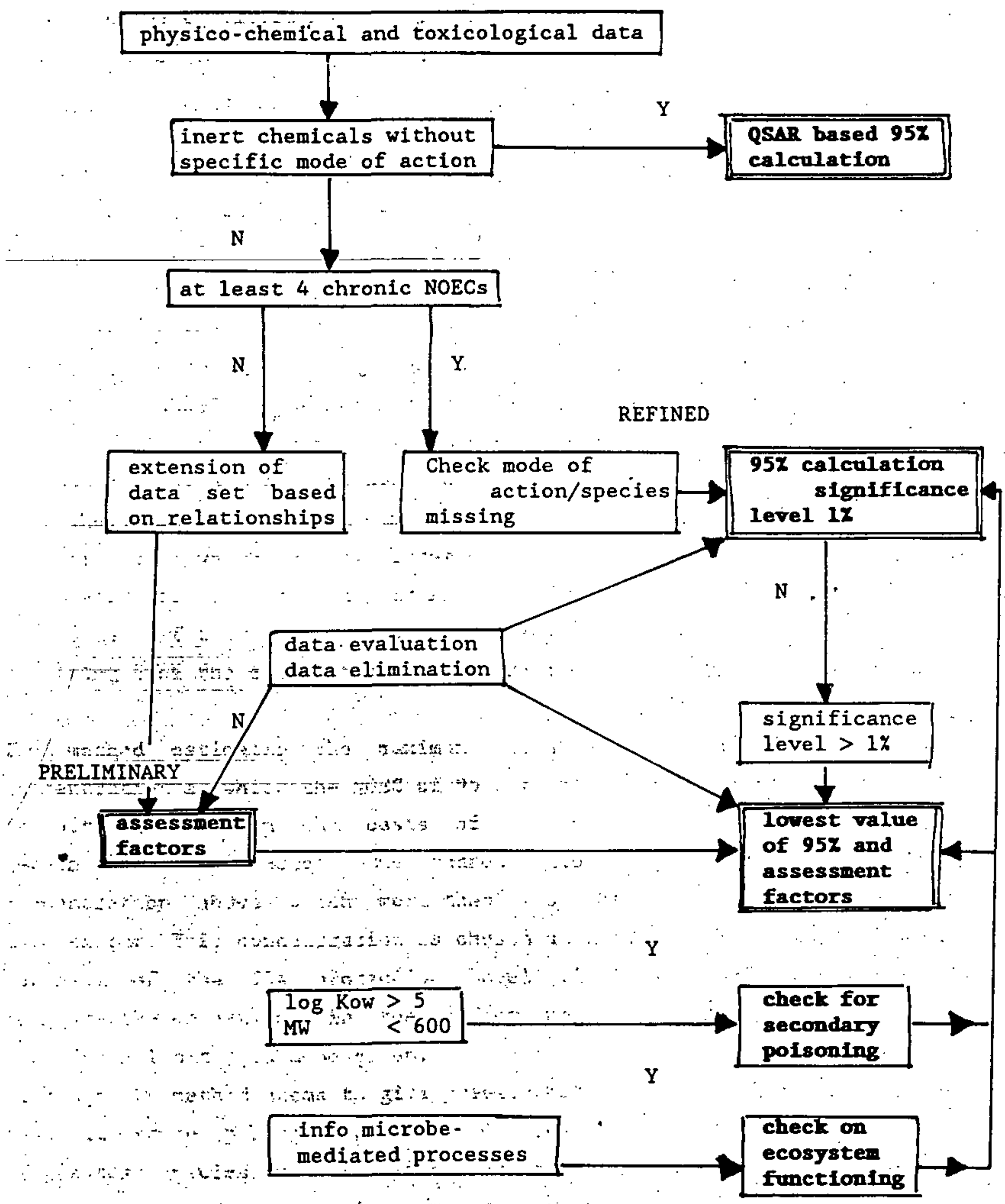


Figure 1: Schematic presentation of ecotoxicological effect assessment of chemical substances for each ecosystem compartment (see text for explanation)

4. REFINED EFFECT ASSESSMENT (the 95% method)

4.1. General aspects

The refined effect assessment procedure is used if sufficient laboratory single species toxicity data are available to derive a maximum tolerable concentration. Data are considered sufficiently available if the data set comprises at least four chronic NOEC-values determined for various species (different in ecological function, anatomic design, route of exposure etc.) in order to meet the species diversity in ecosystems to some extent. However, it should be noted that the availability of data on representatives of the same groups of species as required in the preliminary effect assessment (see 5.2 for example) is not considered conditional. Only in case there are reasons to assume a specific mode of action of the substance as a result of which data on representatives of susceptible species are considered to be essential but missing, the preliminary effect assessment is applied. If there is any doubt both methods are used, the lowest value resulting from the calculations being the maximum tolerable concentration.

The method estimates the maximum tolerable concentration defined as the concentration at which the NOEC of 95% of the species within an ecosystem is not exceeded on the basis of the distribution of experimentally determined NOECs. Hence, the method allows to estimate a critical concentration above which more than 5% of the species may be affected to some extent. This concentration is chosen such that it presents the median estimate of the 95% protection level (lower 50% confidence limit). To indicate the uncertainty in the effect estimation also the lower 95% confidence limit should be given.
Although the method seems to give precise estimates, it should be stressed that it strongly hinges on the assumptions that are made (the NOEC-values of the test species as well as those of the community species are assumed to be conceived of as independent random trials from a log-logistic distribution). Therefore the procedure has to be regarded as a recipe with a rational basis to estimate concentrations of chemical pollutants which may be considered as acceptable. Indications that extrapolation from this

effect assessment procedure on single-species toxicity data yields results that match no-effect levels derived in multi-species experiments have recently been reported by Okkerman et al. (1992) and Emans et al. (1992).

4.2. Calculating 95% protection levels

The method is the result of the historical developments outlined in chapter 2. The method assumes a log-logistic distribution of species sensitivities according to Kooijman (1987), but NOEC values are used instead of LC50 values, which is in accordance with Stephan et al. (1985). Following Okkerman et al. (1992) at least 4 NOEC-values for different species are required. Further the statistics in the method are independent on species number in the ecosystem, being a modification of Van Straalen and Denneman (1989) on the Kooijman's method, but now improved according to the description of Aldenberg and Slob (1992). The procedure is applicable to all environmental compartments and is available on diskette (RIVM-report no. 719102015 by Aldenberg, 1992).

The following steps are distinguished in applying the procedure:

a] Reliable long-term NOEC-values are collected.
It should be noted that the number of long-term toxicity data can be extended.

* In case a reliable compound-specific ratio between a short-term L(E)C50-value and a long-term NOEC for the same test species is available, this ratio may be applied to derive a chronic NOEC for a test species for which only an acute L(E)C50-value is available. This procedure may only be applied between
  [a] different fish species,
  [b] different species of the same genus, and
  [c] any other groups if underpinned by sound arguments. In case several ratios are available the geometric mean ratio is used.
* QSARs may be used to derive maximum tolerable concentrations for chemically related compounds (like the chlorobenzenes, chlorophenols, chloroanalines) if at least for one chemical within such a group a maximum tolerable concentration is available based on experimentally

determined NOEC-values. The maximum tolerable concentrations for the other chemicals in the group is subsequently derived by applying the ratios between the QSAR-values to the maximum tolerable concentration of that chemical. If more QSARs or more experimentally derived maximum tolerable concentrations are available the geometric mean is used.

b] Corrections are made if required (e.g. conversion of sediment and soil data for organic matter and clay content) (***see section 5.4. and chapter 6, point 7***).

c] It is determined whether the toxicity data follow a log-logistic distribution (this assumption has been made by Kooijman and is followed by Aldenberg and Slob). The goodness-of-fit for NOECs is tested using an Emperical Distribution Function Test (available on the diskette, see RIVM report 719102015 by Aldenberg, 1992).
Due to the limited number of data the test is not very powerful and only major deviations from the log-logistic distribution will be detected. Since the power of the test increases with the number of data it may occur especially with large data sets that the test rejects the log-logistic distribution. Therefore the following procedure is advocated:

d] The significance level (1, 2.5, 5 or 10%) is presented at which the test rejects the distribution as being log-logistic (included on the diskette, see RIVM report 719102015 by Aldenberg, 1992).
If the log-logistic distribution of the species sensitivities is not rejected at a level of 1%, the procedure given in e is performed.
- If it is rejected at a significance level of 1% it is unlikely that the species sensitivities are log-logistically distributed. The toxicity data are evaluated based on the knowledge of the mode of action of the compound. There could be a misfitting resulting from outliers. In that case outliers are identified and, if there are reasons to do so, they are eliminated from the input data set. Subsequently the procedure given in f is performed.
- There also could be a rejection due to the fact that the distribution is bi- or multimodal. In that case the most sensitive groups of

species of which the sensitivities do follow a log-logistic distribution are identified and follow the procedure given in f.

- If the species sensitivities are not log-logistically distributed and there are no reasons for leaving out outliers both the results of the refined and preliminary effect assessments are presented. The lowest value is considered as the maximum tolerable concentration.

e] Run the model according to Aldenberg and Slob (1992) as available on diskette (see RIVM report 719102015 by Aldenberg, 1992).

f] Run the model according to Aldenberg and Slob (1992) as available on diskette and motivate the choice of species left out.

4.3. QSAR based 95% protection levels

Experimentally derived NOECs are preferred in establishing maximum tolerable concentrations, but these are not conditional for all compounds. In case there are reliable Q(uantitative) S(tructure)-A(ctivity) R(elationship)-equations for chemicals for a number of test species, these may be applied to derive chronic NOECs. The various classes of chemicals (inert chemicals, less inert chemicals, reactive chemicals and specifically acting chemicals) have been described and listed by Verhaar and Hermens (1991). Currently most QSAR information is available for the inert chemicals.

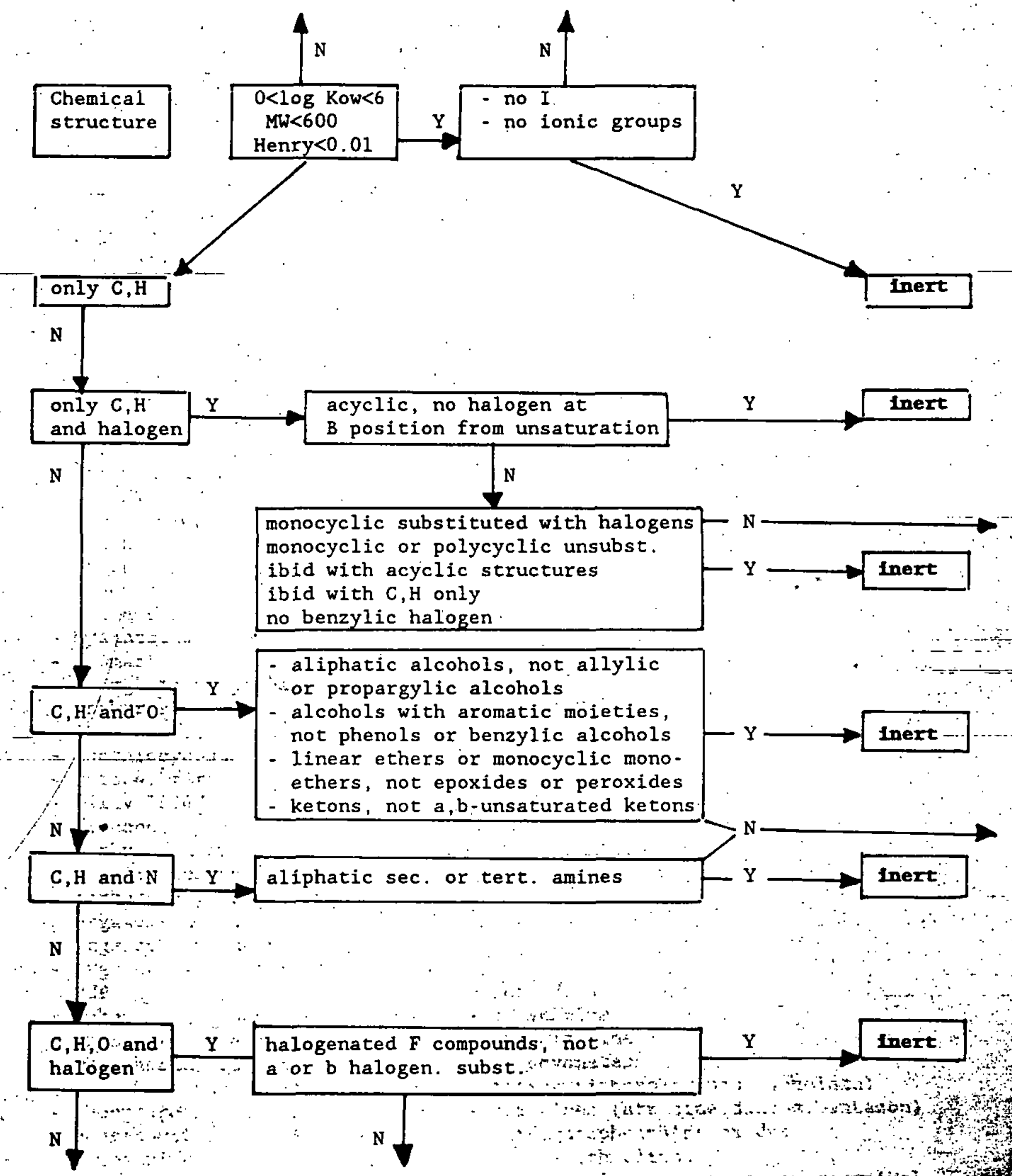
QSARs designed for inert organic chemicals (acting by non-polar narcosis) are based on the K_{ow} and indicate the baseline toxicity of the substance. The baseline NOEC may be used in case there are no indications for specific mode of action.

The following steps are distinguished:

[a] Classification of the chemicals. Structural requirements for chemicals exerting non-polar narcotic action are currently restricted to organic compounds that consist of carbon, hydrogen, nitrogen, oxygen and/or halogens (iodine excluded). These chemicals can be classified as such according to the flow scheme given in figure 2.

[b] Checking for specific mode of action. Some of the chemicals are known to exert a specific mode of action. These chemicals are listed in table 2.

[c] If the chemicals are classified as inert chemicals and no specific mode of action is known, the calculated maximum tolerable concentrations of this type of chemicals in water and sediment may be derived according to Van Leeuwen et al. (1991) as presented in table 3 for chemicals with log K_{ow}-values ranging from 0 to 6. The maximum tolerable concentrations in the soil are set equal to those derived for the sediment, whereas those for the air are derived based on information on the Henry coefficient of the compound (see 3.2.b). (***see chapter 6, point 8***)



<u>Figure 2</u>: Classification scheme for classifying inert chemicals (after Verhaar and Hermens, 1991)

Table 2: Chemicals that may be classified as inert chemicals according to flow scheme A, acting by a specific mechanism (Verhaar and Hermens, 1991)

- alkyl/aryl-dodecadienoates
- aromatic sulphonates/sulphonate esters
- atropin and analogues (tropates)
- (aziridine)phosphide oxydes
- (aziridine)phosphide sulphides
- barbiturates
- (benzene/toluene)sulphonamides
- benzimidazoles
- benzoylphenylureas
- biogenic lactones (avermectins)
- bipyridilium derivates (diquat, paraquat)
- camphenes
- carbamates
- cyanates
- DDT and analogues (DDD, DDE, DDMU)
- (di)phenylacetic acid derivates
- dialkyl)formamidines
- dinitrophenols
- (dioxo)pyrazolidines
- drins
- ether derivates of hydroxyacetic acid
- griseofulvin
- hydantoins
- coumarins
- inorganic propionates
- isobornanes
- isocyanates
- isothiocyanates
- kepone, mirex
- Lilly 18947
- lindane
- methylenedioxobenzenes
- nicotin analogues
- norbornanes/norbornenes
- organometallics
- organophosphate esters
- organophosphorothionate esters
- PCP
- (pheno)thiazines
- phosphate esters
- phosphoric triamides
- phosphorocyanidates
- phosphorofluoridates
- phosphorotrihioites
- piperazines
- pyrethroids
- chrysanthemates
- SKF-525 A
- strychnine
- sulphinimides
- thiocyanates
- triazatriphosphorines (apholate)
- triazines (atrazine,diuron,bentazon)
- triorganophosphine oxydes
- (1,2)-dithiolanes
- 2-phenyl-3-pyrazolones (aminopyrine)
- (2-thione) thiadiazines

Table 3 95% protection levels in surface water and sediments for inert organic chemicals without specific mode of action (Van Leeuwen et al., 1991). Those for groundwater and soil may be derived as presented in chapter 5. The 95% protection level for air may be derived based on the Henry coefficient (Kp water/air).

Log Kow	dissolved (mol/l)	sediment (mol/kg)	Log Kow	dissolved (mol/l)	sediment (mol/kg)
0.0	-2.97	-4.50	3.0	-5.89	-4.41
0.1	-3.06	-4.48	3.1	-6.00	-4.42
0.2	-3.15	-4.47	3.2	-6.10	-4.43
0.3	-3.23	-4.46	3.3	-6.21	-4.43
0.4	-3.32	-4.45	3.4	-6.32	-4.44
0.5	-3.41	-4.44	3.5	-6.42	-4.45
0.6	-3.50	-4.43	3.6	-6.53	-4.46
0.7	-3.60	-4.42	3.7	-6.64	-4.46
0.8	-3.69	-4.41	3.8	-6.75	-4.47
0.9	-3.78	-4.40	3.9	-6.86	-4.48
1.0	-3.88	-4.40	4.0	-6.97	-4.49
1.1	-3.97	-4.39	4.1	-7.08	-4.50
1.2	-4.07	-4.39	4.2	-7.19	-4.51
1.3	-4.16	-4.38	4.3	-7.30	-4.52
1.4	-4.26	-4.38	4.4	-7.41	-4.53
1.5	-4.36	-4.38	4.5	-7.52	-4.54
1.6	-4.45	-4.38	4.6	-7.63	-4.55
1.7	-4.55	-4.38	4.7	-7.74	-4.56
1.8	-4.65	-4.38	4.8	-7.85	-4.57
1.9	-4.75	-4.38	4.9	-7.96	-4.59
2.0	-4.85	-4.38	5.0	-8.08	-4.60
2.1	-4.95	-4.38			
2.2	-5.06	-4.38			
2.3	-5.16	-4.38			
2.4	-5.26	-4.39			
2.5	-5.37	-4.39			
2.6	-5.47	-4.39			
2.7	-5.57	-4.40			
2.8	-5.68	-4.40			
2.9	-5.78	-4.41			

4.4. Secondary poisoning

Once emitted, chemical substances are distributed between solid (sediment, soil), liquid (surface water, groundwater, rain water) and the gaseous (air) phases of the environment. Some chemicals, however, may also accumulate in biota. This especially counts for some heavy metals and organic compounds with a relatively high K_{ow} and relatively low molecular weight. When contaminated biota is preyed upon by predatory species, the

predators are exposed to chemicals present in their prey as well. The uptake of chemicals through water, soil and air may lead to primary poisoning (if the environmental concentration > NOEC); the uptake of chemicals through ingestion of food may lead to secondary poisoning (concentration in food > NOEC of predator). Hence, to avoid secondary poisoning the concentrations of chemical substances in the food should be below the NOEC in dietary toxicity test with animals representative for predators. So far attention has been limited to higher organisms: the birds and mammals. The reason for this is that these groups of higher organisms are at the top scale of the food chain and therefore may be considered as groups at risk. Moreover special attention is given to these groups as a number of them have been placed on the "attention species list" in the nature reservation policy framework. In practice this means that in the derivation of the maximum tolerable level the neglectibility of the risk of adverse effects in these species should be accounted for.
The following steps are distinguished in including secondary poisoning in the derivation of the maximum tolerable concentration:

[a] Based on its physico-chemical characteristics it is determined whether the compound has bioaccumulative potential. Organic compounds are expected to bioaccumulate significantly if log K_{ow} > 5 and molecular weight <600.

[b] If the compound is considered to be potentially bioaccumulative, the BCF-value (both the mean and maximum value) is determined as described in section 3.2.b. To minimize the effort initially only review articles are used to determine the geometric mean and maxima.

[c] Toxicological input data for birds and mammals are determined as described in section 3.2.b. The toxicity data are combined unless the data indicate a difference in susceptibility between birds and mammals. To minimize the effort initially review articles are used only. Sub-acute (< 1 month exposure) NOECs are extrapolated to chronic NOECs by applying a factor of 1/10 (Romijn et al., 1991a). Often toxicity data are expressed in mg/kg bw instead of in mg/kg food. In table 4 conversion factors are given for the most commonly used test species.

Table 4. Conversion factors for toxicity values expressed in mg/kg bw to values in mg/kg food intake

Species	Conversion factor (bw/dfi)
Birds	
Anas platyrhynchos (mallard duck)	9.8
Colinus virginianus (bob-white quail)	4.5
Coturnix coturnix japonica (Japanese quail)	8.7
Gallus domesticus (chicken)	5.7
Passer domesticus (house sparrow)	1.2
Phasianus colchicus (ring-necked pheasant)	9.8
Streptopelia risoria (ringed turtle dove)	11
Mammals	
Blerina brevicauda (short-tailed shrew)	8.0
Canis domesticus (dog)	40
Felis domesticus (cat)	20
Macaca mulatta (rhesus monkey)	20
Mus musculus (mouse)	8.3
Mustela vison (mink)	10
Oryctolagus cuniculus (rabbit)	33
Rattus norvegicus (laboratory rat)	20

[d] Distinction is made between the aquatic and the terrestric food chain:

- Aquatic food chain:
  In aquatic food chains chemicals that have bioconcentration potential (a high BCF) may result in secondary poisoning (Romijn et al., 1991a). The NOECs derived for birds and mammals are divided by the geometric mean BCFs and maximum BCFs resulting in NOECs for fish and mussel eating birds and mammals expressed as NOECs in surface water. The most critical exposure route is chosen.
- Terrestric food chain:
  In terrestrial food chains the bioconcentration potential is not considered critical in excerting secondary poisoning, but the difference in susceptibility between the soil organism and its predator is (Romijn et al., 1991b). Yet the same procedure is followed: the NOECs derived for birds and mammals are divided by the mean and maximum BCF-values, 1 and 10 respectively, resulting in NOECs for soil invertebrate eating birds and mammals expressed as NOECs in soil.

[e] - Aquatic food chain.

* In case there are at least four chronic NOECs for different aquatic species (see 4.2.) the converted NOECs for birds and mammals are added to the data set derived for aquatic species and used as input data in the procedure described in section 4.2.c.
* In case the number of chronic NOECs is insufficient for applying the refined effect assessment, or if there is no NOEC for birds or mammals but LC50s, or a combination of both, the preliminary effect assessment is followed (chapter 5).

- Terrestric food chain.

For the terrestric food chain a similar procedure is followed.

[f] Subsequently it is examined whether the "attention species" are sufficiently protected at the 95% protection level. Hereto the obtained 95% protection level is compared with the NOEC-values derived for predatory birds and mammals on the basis of both the geometric mean and the maximum BCF. In case the NOECs of predatory species are lower than ten times the derived 95% protection level concentration, detailed literature studies are performed into the BCFs and the toxicity to birds and mammals and the exercise is repeated with more accurate data.

In case the (more accurate) NOECs of predatory species are lower than the (more accurate) concentration corresponding to the 95% protection level do not necessarily result in adjustment of the maximum tolerable concentration as such. Toxicity data on "attention species" are lacking in most cases, enforcing the use of toxicological information on non-related species that is available. Taking into account the consequent uncertainties in the estimates of NOECs of the "predators" the information only indicates the possibility for effects in the top of the food chain; the ultimate choice of MPL is a political matter.

4.5. Ecosystem functioning

The ecotoxicological knowledge exists mainly in the field of effects of toxic chemicals on the individual level of a species. As a result the followed effect assessment methodology is based on the limited information at which environmental concentration the survival, growth or reproduction of the average individual of a species will not be affected. The assumption that protection of ecosystem strucure also entails the protection of ecosystem functioning is theoretically debatable (National Health Council, 1989). Therefore information that is not specifically species-related but that is related to the functioning of a group of species (for example effects on microbe-mediated processes like respiration, ammonification, mineralization etc. that is often available for soil ecosystems) should be used in the effect assessment as well. Usually process parameters are sum parameters; they may very well be less sensitive than the other toxicological endpoints measured in single species as the functioning of susceptible species may be taken over by less susceptible species (Van Beelen et al., 1991).

As described in chapter 5 the results of studies on the functioning of groups of species is included in the preliminary effect assessment for soil. Since one aims at the protection of species an assessment factor of 10 is applied to the lowest NOEC determined for microbe-mediated processes to protect ecosystem functioning.
In the refined effect assessment procedure data on functional endpoints (if there are at least 4 chronic NOECs) are treated in the same way as decribed for the structural endpoints, resulting in a concentration at which the NOEC of 95% of the functions is not exceeded.

Subsequently the result is compared with the 95% protection level calculated from single-species toxicity data as described in 4.2. Both the results of the calculations of the concentrations at which species and processes are sufficiently protected are presented.

5. PRELIMINARY EFFECT ASSESSMENT (the 10x10x10 method)

5.1. General aspects

The preliminary effect assessment procedure is applied in case insufficient data are available to estimate a maximum acceptable level with the refined procedure. Information is considered insufficient in case less than four chronic NOEC-values are available for different species (different in function, structure, route of exposure etc. in order to meet the species diversity spectrum in ecosystems to some extent). Hence, the method allows to make an indicative judgement of the ecotoxicological properties of a substance even if only one acute LC50 or acute QSAR-estimate is available.
The preliminary effect assessment procedure is based on the results of the OECD-workshop held in December 1990. The result obtained by applying this procedure is to be considered as a tentative (ecotoxicological advisory) value and may be referred to as an indicative maximum tolerable concentration.

The method has no scientific basis: it assumes a constant and identical difference (a factor of 10) between chronic and acute toxicity, and between single-species and ecosystem sensitivity. The lowest toxicity value of concern is divided by an assessment factor of which the extent (varying from 10-1000 based on the 10x10x10 principle) decreases with increasing information on the ecotoxicity of the substance.

The following procedure is followed:
- If the required information is only partly present (e.g. two acute LC50s and one chronic NOEC) the lowest value obtained upon application of the various factors (10, 100, or 1000 to the information concerned) is considered the indicative MTC.
- If a group of structure related compounds is considered and QSAR estimates are available, QSAR information is used. In case more than one QSAR estimate is available the geometric mean of the QSARs is used.
- Chronic NOEC may be estimated from acute data as described in section 4.2.a.

Below the procedure is outlined specifically for each environmental compartment.

5.2. Surface water

Aquatic toxicology is the most developed area in ecotoxicology. The activities in the last decades have resulted in a large amount of data, mostly concerning algae, Daphnia and fish. However, for many compounds less than 4 chronic toxicity data are available and subsequently the preliminary effect assessment procedure is used. Hereto the information on aquatic toxicity data and the subsequent assessment factors are presented in table 5.

Table 5: Preliminary effect assessment procedure for surface water (for explanation see 5.1)

Information available	*Assessment factor*
Lowest acute L(E)C50 or QSAR-estimate of acute toxicity	*1000*
Lowest acute L(E)C50 or QSAR-estimate for at least representatives of algae, crustaceans and fish	*100 **
*Lowest chronic NOEC or QSAR-estimate for at least representatives of algae, crustaceans and fish ***	*10 **

** Lowest value is selected in case < 3 chronic NOECs are available*
*** MicroTox data may be used*

5.3. Sediment

The development of sediment toxicology has been initiated just a few years ago and therefore toxicity data on sediment inhabiting organisms are rare. In fact three different methods may be applied to derive an indicative maximum tolerable concentration in sediment, partly based on the recommendations of the international workshop in Copenhagen on Effect Assessment of Chemicals in Sediment (1991):

[a] Sediment toxicity testing

This method is analogous to the derivation of maximum tolerable concentrations for surface waters. If data are available a normalization procedure (see 5.4.) is applied to overcome the large sediment-to-sediment variations. However, sediment toxicity testing is still in development and toxicity data on sediment inhabiting organisms are rare. Although this method is preferred, it has little practical value at this moment.

[b] Equilibrium partitioning method

In this method the indicative maximum tolerable concentration in the sediment is based on the value derived from the maximum tolerable concentration determined for surface water, according to the equilibrium-partition method described by EPA (1989). Application of this method has been presented by Van der Kooy et al. (1991). In the method it is assumed that:

- sediment-dwelling organisms and water column organisms are equally sensitive to the chemical,
- concentrations in sediment, interstitial water and benthic organisms are at thermodynamic equilibrium: concentrations in any of these phases can be predicted from one another using the appropriate equilibrium partitioning constants,
- sediment-water equilibrium partition constants can be derived on the basis of a generic partition model from separately measurable characteristics of the sediment and properties of the chemical.

The formula used is:

$MTC_{sed} = K_p * MTC_{wat}$, where

MTC_{sed} = MTC in sediment [$mg.kg^{-1}$ dry sediment]

MTC_{wat} = MTC in water [$mg.l^{-1}$ water]

K_p = partition coefficient (l water.kg^{-1} sediment)

For metals no generic partition model is available (see also table 1). The median values as presented in table 1 may be used to derive a maximum tolerable concentration in the sediment. Laboratory experiments indicate, however, that metal toxicity in sediments is suppressed completely if amorfous iron sulfide, measured as Acid Volatile Sulfide (AVS) is present in a molar concentration higher than the sum of the molar concentrations of metals for which the solubility of the sulfide is less than the solubility of iron sulfide (Zn, Cd, Ni, Pb, Cu, etc.) (DiToro et al., 1991; 1992). Thus, the AVS concentration of a sediment establishes the boundary below which these metals cease to exhibit toxicity in freshwater and marine sediments. Following the OECD-guideline, the MTC_{sed} for the sum of metals is set equal to the AVS-content of the sediment:

$$MTC_{sed}[Zn+Cd+Ni+Pb+Cu+Cr+Hg] = AVS$$

(**chapter 6, point 9**).

[c] The value derived from the maximum tolerable concentration determined for standard soil based on soil toxicity data. It should be noted that this method was not recommended by the OECD but is based on the environmental policy approach in The Netherlands that no distinguishment is made in standard setting between land soils and sediments.

No generic guide can be given which value should be preferred or how to evaluate them; the ultimate choice being highly dependent on the amount, nature and reliability of the data.

5.4. Soil

Basic efforts in developing soil toxicity testing were started 10-15 years ago. As a result only few soil toxicity data are available mostly dealing with effects on microbial processes and earthworms. For this reason information on effects on processes mediated by micro organims is included in the procedure, whereas initially this is not the case in the refined effect assessment method. Two methods may be used:

[a] Soil toxicity testing

In analogy with the method for sediments toxicity data are normalized. (*see chapter 6, point 7)*

. For organic compounds, normalization is based on the organic carbon content of the soil:

$NOEC_{standard} = NOEC_{exp} * f_{oc}(standard)/f_{oc}(experiment)$,

with f_{oc}(standard) = 5% (which is about 10% organic matter)

. For metals toxicity data are normalized for organic matter and clay content valid for standard soil (organic matter 10%; clay 25%):

$NOEC_{standard} = NOEC_{exp} * R\ (25,10)\ /\ R_{exp}(L,H)$

where

R = reference value for standard soil: value calculated by using a clay content of 25% and an organic matter content of 10%

R_{exp} = value determined for the experimental soil, calculated by using the clay (L) and organic matter (H) content of the soil used in the experiment

Although not meant for this purpose, the formulas for application of Soil Reference Values (VROM, 1990) are used:

Chromium	[Cr] = 50 + 2 L	R = 100	$mg.kg^{-1}$
Nickel	[Ni] = 10 + L	R = 35	$mg.kg^{-1}$
Lead	[Pb] = 50 + L + H	R = 85	$mg.kg^{-1}$
Copper	[Cu] = 15 + 0.6 (L + H)	R = 36	$mg.kg^{-1}$
Arsenic	[As] = 15 + 0.4 (L + H)	R = 29	$mg.kg^{-1}$
Zinc	[Zn] = 50 + 1.5 (2L + H)	R = 140	$mg.kg^{-1}$
Cadmium	[Cd] = 0.4+ 0.007 (L +3H)	R = 0.8	$mg.kg^{-1}$
Mercury	[Hg] = 0.2+ 0.0017 (2L + H)	R = 0.3	$mg.kg^{-1}$
Barium	[Ba] =300 + 3.9 L	R = 200	$mg.kg^{-1}$
Cobalt	[Co] = 10 + 0.17 L	R = 20	$mg.kg^{-1}$

Subsequently a procedure analogous to that proposed for surface water is applied (see table 6). Although it is realized that only few QSARs are available (e.g. Van Gestel et al., 1991), QSARs are included in the table for reasons of consistency.

Table 6: Preliminary effect assessment procedure for soil (for explanation see 5.1)

Information available	*Assessment factor*
Lowest acute L(E)C50 or QSAR-estimate of acute toxicity	*1000*
Lowest acute L(E)C50 or QSAR-estimate for at least three representatives of microbe-mediated processes, earthworms or arthropods and plants	*100 **
Lowest chronic NOEC of QSAR-estimate for at least three representatives of microbe-mediated processes, earthworms or arthropods and plants	*10 **

** Lowest value is selected in case < 3 chronic NOECs are available*

[b] Equilibrium partitioning method

In case no soil toxicity data are available the equilibrium partition method described in 5.3.b is used.

5.5. <u>Groundwater</u>

Toxicity data on groundwater inhabiting organisms are lacking and it is only recently that groundwater obtained attention by ecotoxicologists (Van Beelen et al., 1991; Notenboom et al., in preparation). Therefore the indicative maximum tolerable concentration is determined by

[a] the value equal to the maximum tolerable concentration determined for surface water,

[b] the value derived from the maximum tolerable concentration determined for soil, according to the equilibrium-partition method described by EPA (1989): the reverse of the procedure described in 5.3.

No generic guide can be given which value should be preferred or how to evaluate them; the ultimate choice being highly dependent on the amount, nature and reliability of the data.

5.6. Air

As to the air compartment toxicological data on animal species other than mammals are usually not or only scarcely available (***see chapter 6, point 10***) . Taking into account that one aims at the protection of man at the level of the individual instead of the level of populations of species as is the case with ecosystems, it may be assumed that the maximum tolerable concentrations for humans will be sufficiently restrictive in protecting other species in most cases (as result of applying larger assessment factors). However, some species are more vulnerable than man. Attention should be paid to birds since [a] they have a higher ventilation rate, [b] they have a respiratory system that differs markedly from that of mammals, [c] they may be exposed to relatively high pollutant concentrations over long periods of time and [d] they may have a different metabolism. This may also hold for insects. Plants may be more susceptible than animal species, having a totally different physiology and biochemistry, and therefore should be included in the test battery. Being totally dependent on the atmosphere special attention should be given to lichens. In table 7 a tentative procedure to estimate an indicative maximum tolerable concentration is proposed. Literature data are corrected for a full time exposure: 24 hours a day and 7 days per week, applying the following formula: LC50 or NOEC = $LC50_{exp}$ or $NOEC_{exp}$ * d/7 * h/24, in which d = number of days exposed per week and h = number of hours exposed per day.

Table 7: Preliminary effect assessment procedure for air (see 5.1)

Information available	*Assessment factor*
Lowest acute L(E)C50 (or QSAR-estimate) of acute toxicity	*1000*
Lowest acute L(E)C50 (or QSAR-estimate) for at least three representatives of mammals or birds, plants or lichens, and insects	*100 **
*Lowest chronic NOEC (or QSAR-estimate) for at least three representatives of mammals or birds, plants or lichens, and insects ***	*10 **

* *Lowest value is used in case < 3 chronic NOECs are available*
** *Sub-acute data for birds and mammals (< 1 month) are extrapolated to chronic data by applying an extra factor of 10*

5.7. Food (biomagnification)

Food plays an important role in the total intake of biomagnifying substances. This especially counts for predatory birds and mammals. In analogy with the procedure outlined in chapter 4 the results based on direct exposure to the abiotic environment are compared with the maximum tolerable concentration based on the prevention of secondary poisoning. This comparison indicates the degree in which predatory birds and mammals are protected. In case insufficient data are available to estimate acceptable concentrations for predators, the assessment factors as presented in table 8 may be applied.

Table 8: Preliminary effect assessment procedure for birds and mammals via the food chain (see 5.1)

Information available	*Assessment factor*
Lowest acute L(E)C50 (or QSAR-estimate) of acute toxicity	*1000*
Lowest acute L(E)C50s (or QSAR-estimate) for at least three species representing both bird or mammalian species	*100 **
*Lowest chronic NOECs (or QSAR-estimate) for at least three species representing both bird or mammalian species ***	*10 **

* *Lowest value is selected in case < 3 chronic NOECs are available*
** *Sub-acute data (< 1 month) are extrapolated to chronic data by applying an extra factor of 10*

6. CURRENT ACTIVITIES AND FUTURE NEEDS

6.1. Toxicological endpoints

From a scientific point of view it is recognized that it is very difficult to determine which toxicological endpoints are relevant to be studied in relation to the existance of species. Recently the Health Council of the Netherlands selected 24 quality parameters to enable the effects of toxic chemicals on soil and sediment ecosystems to be assessed (Health Council, 1991). Although scientists may encourage the use of all these parameters, practice learns that the data availability for most chemicals is restricted to test parameters required in legislative frameworks. Further research is needed into the necessity and the feasibility of requiring the testing of additional toxicological endpoints.

6.2. Alternatives for the NOEC

There are arguments against the NOEC as a basis from which to start extrapolation from single-species level to the level of higher biological organization. Major disadvantages of the NOEC-concept are that the derivation of the NOEC is determined by the differences in test concentrations and that the experiment very well may have been too small to observe differences in response. In this respect Hoekstra and Van Ewijk (1992) advocated the use of a model free estimation of the concentration with a limited bounded effect (e.g. 25%) followed by linear extrapolation to a concentration with an acceptable effect (e.g. 5%). From a scientific point of view it is recommended to adopt the proposal of Hoekstra and Van Ewijk (1992), and to discuss the advantages both nationally and internationally. It should be recognized, however, that there will be reluctancy due to the fact that most toxicity data available are expressed as NOEC-values, being derived according to internationally accepted test method protocols.

6.3. Geometric mean vs. median values

Since a log-logistic distribution of species susceptibilities is assumed, a geometric mean is used instead of a median value. In order to be consistent also the geometric mean is used in case of bioconcentration factors and partition coefficients. This may be subject to further discussion.

6.4. Clustering of toxicity data

Van de Meent and co-workers (1990) suggested to cluster single species toxicity data taxonomically. Reason was

a] the assumption that phylogenetically related species show more similarity in toxicant susceptibility than non-related species, and

b] literature toxicity data doesn't necessarily correspond with a random sample of species from an ecosystem.

In this document no clustering was performed as at this stage there is no full agreement for clustering toxicity data to a certain taxonomic level higher than the species level. It is felt that this aspect needs further attention and it has been subject for recommendation by the Health Council earlier (1991). As a part of the project ECO-effects the RIVM has initiated a study into the sensitivity patterns of species to toxicants in order to derive quantitative species sensitivity relationships (QSSRs). The information gathered from this project may provide a basis for clustering groups of species (Hoekstra et al., 1992).

6.5. Coordination of maximum tolerable levels soil/sediment

The consequence of using different pH levels for sediment and soil is that the maximum tolerable concentration of a substance in soil not necessarily matches the maximum tolerable concentration in sediment. This is not coherent to the approach of the environmental policy in setting standards for substances in sediment and soil. This problem needs further attention.

6.6. Bioconcentration and secondary poisoning

The development of methods to determine the possible impact of secondary poisoning has just started. In the coming years attention will be given to the effects of biomagnification along different lines:

[a] the development of a boxmodel system containing various modules representing groups of biological species with a similar way of

exposure. For example attention will be paid to the transfer of chemicals from soil/litter -> plants -> insects -> birds -> birds of prey. This activity will largely be carried out by the RIVM as a part of the project ECO-routing.

[b] In depth studies into (i) the bioavailability of the chemical in the food/prey (the bioavailability may be very well less in the field compared to results obtained in laboratory experiments), (ii) the food conversion factors (different food may have different caloric value, resulting in different amount of daily food), (iii) efficiency of food consumption (different species may have different efficiencies; specialists may show a higher efficiency), and (iv) the metabolic activity (there may be differences in metabolic activities within one species between field and laboratory conditions, as well as in the field through the seasons). This activity will largely be performed by DGW, focused on the marine environment, in collaboration with RIVM (ECO-routing; other compartments) (Everts, 1991).

[c] The information gathered from [a] and [b] will be tested and used in an Ecosystem Model (Aldenberg and Traas, 1991) on a substance by substance and ecosystem by ecosystem base by the RIVM as part of the project ECO-rendement.

6.7. Corrections for soil and sediment characteristics

According to the environmental policy normalization of soil and sediments is required (DGM, 1991). Conversion of the data of different soils to a standard soil is performed for clay content and organic carbon content. This conversion is based on the findings of the VTCB (1986) relating soil characteristics and metal concentrations in nature reserves ("background values"). The conversion is applied to determine effect concentrations since association with bioavailability was indicated. However, earlier it has been doubted whether the described relationships between the percentage of OC and/or the percentage of clay in the soil and the presence of metals is dominantly associated with the bioavailability and therefore with the toxic effects of the metals (Van de Meent et al., 1990). The report of WL (1991) on standard setting in marine sediments led to new discussions. In marine sediments the OC and clay contents are related and this may very well be the case in land soils. If so, the use of only the OC or the clay content is needed, simplifying the standard setting and control measures. In fact the total normalization procedure as such may be subject to evaluation since preliminary results indicate that correction factors do not deviate much from 1 based on the normal range of OC and clay contents in the Netherlands.

6.8. Deriving MTCs for air from those for water

Concentrations of a substance in the various environmental compartments are interrelated. Under constant environmental and emission conditions all environmental concentrations will become constant in time. Based on the characteristics of the environment and the substance one may estimate the concentration in the air from that in water by using the Henry coefficient. This has been discussed at a Workshop on "Integrale Normstelling Stoffen" (Van de Meent et al., 1991). The approach will be evaluated by the RIVM as a part of the project ECO-routing. It should be noted that applying this method only the baseline toxicity is derived; effects on organisms exposed to pollutants in air may result in lower NOEC-levels. This especially counts for chemicals that are harmful to plants.

6.9. Bioavailability of heavy metals in Dutch sediments

The AVS-model has not been validated in The Netherlands and AVS-contents of Dutch sediments are yet not even known. Rough estimates indicate that metal toxicity in Dutch sediments may very well be controled by sulphide solubility, instead of equilibrium partitioning. This topic will be studied as a part of the project ECO-routing by the RIVM and by RIZA.

6.10 Lack of ecotoxicological information air pollutants

The amount and nature of information of effects of chemical substances to animals and plants when exposed through air is very limited. Where the ecotoxicological effects of aquatic pollutants have been subject to study for decades and those of soil pollutants have gained much interest in the last 10-15 years, no such development takes place for air pollutants. This has been recognized by the Health Council (1989): "the committee states that there is a lack of sound, accepted and standardized tests for the compartment(s) (soil and) air; this applies to both acute and chronic tests. The committee considers this a very serious matter". The need for initiating efforts to come to ecotoxicological testing and evaluation of air pollutants was stressed at the 3rd US-Dutch expert Workshop on Comparative Risk Analysis for Air Pollution Prevention (Slooff and Tingey, 1991), as well as at the Workshop on "Integrale Normstelling Stoffen" (Slooff, 1991), and still stands today.

6.11 <u>Combined toxicity</u>

The outlined procedure only derives a MTC based on observations of the effects of a single chemical compound; no attention has been given to effects resulting from exposure to mixtures of chemicals. Practice learns that synergism is rare and recent evidence indicates that low sub-lethal concentrations of a chemical may still excert a harmful effect when present in a mixture. It is assumed that (partial) additive joint action does occur. Hence, this phenomenon could be incorporated into the derivation of a MTC, e.g. based on a simple concentration addition approach based on site-specific information on chemical pollution. However, one may also argue that the desirable level (1% of the MTC for xenobiotic substances or the background value for natural compounds) is considered to be sufficiently protective in general.

6.12 <u>Validation</u>

It should kept in mind that maximum tolerable concentrations as determined in this report are solely based on the results on standardized laboratory toxicity tests on a very small fraction of species in natural ecosystems. In nature the conditions and species composition will vary in time and space, and so will the ecosystem susceptibility. Therefore further validation of the results of the effect assessment is urgently needed. In immitation of the validation projects on freshwater ecosystems (Emans, et al., 1992) a validation project on soil ecosystems will be inititiated in 1992 by the RIVM in collaboration with other research organizations.

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