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GUIDANCE DOCUMENT ON THE DERIVATION OF ECOTOXICOLOGICAL CRITERIA FOR SERIOUS SOIL CONTAMINATION IN VIEW OF THE INTERVENTION VALUE FOR SOIL CLEAN-UP

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1. INTRODUCTION

In the framework of the periodical revision of the Soil Protection Guidelines in the Netherlands, and incorporation of the Interim Soil Clean Up Act in the Soil Protection Act, intervention values (formerly C-values) have been derived. Exceedance of the intervention value means "serious soil contamination", an unacceptably increased risk to man or the environment, taking into account all possible exposure pathways (VROM, 1990). In principle there is a "need for clean-up". A subsequent actual risk analysis determines the priority for clean-up. The intervention value for soil clean-up is based on the integration of a separately derived human-toxicological- as well as an ecotoxicological criterium for serious soil contamination (van den Berg et al., 1993).

This report concerns the methodology used to derive the ecotoxicological criteria for serious soil contamination. The methodology used to derive the human-toxicological criteria will be described in report nr. 950011 004 (Janssen, 1995). The history of the ecotoxicological criteria for serious soil contamination starts in 1990 with the publication of an RIVM-report by Denneman and van Gestel (1990). In the mentioned report the criterion "serious danger for functional aspects of soil ecosystems" was elaborated and proposals were done for ecotoxicological criteria. In a supplementary report (Denneman and van Gestel, 1991) these values were compared with values derived through equilibrium partitioning using aquatic toxicity data.

The startingpoint of the ecotoxicological criterium is that there is a serious danger for an ecosystem when the ecological functioning of the ecosystem is threatened (Denneman and van Gestel, 1990). It is assumed that this will be the case when the structure of an ecosystem is threatened by an affection of the species diversity. The ecotoxicological criterium for serious soil contamination is that there is a serious danger for a soil ecosystem when 50% of the species and 50% of the microbial processes are threatened. This will be the case when the NOEC (No-Observed-Effect-Concentration) for effects on vital life-functions of species, (like survival, growth and reproduction) and microbial- and enzymatic processes are exceeded expressed as the Hazardous Concentration for 50% of the species or microbial processes (HC50).

Both the reports of Denneman and van Gestel (1990, 1991) have been evaluated by the Technical Soil Protection Committee and recommendations have been given (TCB, 1992). Since the publication of Denneman and Van Gestel, new knowledge has become available, concerning some of the topics mentioned in the recommendations of the Technical Soil Protection Committee.

The aim of this document is to update the methods described by Denneman and Van Gestel with recommendations given by the Soil Protection Committee and with scientific information and methods which have become available in recent years. Besides this there is a strong need to describe the methodology in a stepwise procedure, to facilitate the derivation of future ecotoxicological criteria for serious soil contamination.

The methodology used to derive ecotoxicological criteria for serious soil contamination is described in a stepwise protocol. A schematic summary of the protocol is presented in Chapter 2. The protocol itself is presented in

Chapter 3. The different steps of the protocol give guidance on the data to be collected and the corrections and calculations to be performed to derive HC50-values and in the end the ecotoxicological criterium for serious soil contamination. The definitions of the different HC50-values in the protocol are given in Appendix I. Each step in the protocol also contains so-called BOXES, containing a summary of the scientific background with references. These BOXES can be consulted when necessary.

It has to be kept in mind that the protocol presented is a composition of the methods and knowledge available at this moment. The stepwise approach makes it possible to identify the methods used and the uncertainties introduced. This means that new knowledge that will be available in the future can be incorporated. Comments on and recommendations to improve this protocol are therefore welcome.

2. SCHEMATIC PRESENTATION

A schematic presentation of the protocol is shown in Figure 1. If a relative large data base is available, statistical extrapolation methods are used to derive HC50-values for species and microbial processes (Hazardous Concentration for 50% of the terrestrial species or microbial processes). These methods are commonly used in the Netherlands for deriving environmental-quality guidelines for water, air, sediment and soil.

The procedure can be divided in two subprocedures. In subprocedure I the criterium for serious soil contamination is derived using toxicity data on terrestrial species. In subprocedure II the equilibrium partition method is applied. By using the equilibrium partition method the toxicity for soil organisms is predicted from toxicity data on aquatic organisms.

Whether subprocedure I and/or subprocedure II is applied depends on the amount of terrestrial data available (Figure 2). If enough terrestrial toxicity data are available, subprocedure I determines the criterium. If only few terrestrial toxicity data are available subprocedure II is also applied. If no terrestrial toxicity data are available, it is only possible to apply subprocedure II. The subprocedure(s) used gives also an indication of the reliability of the ecotoxicological criterium for serious soil contamination.

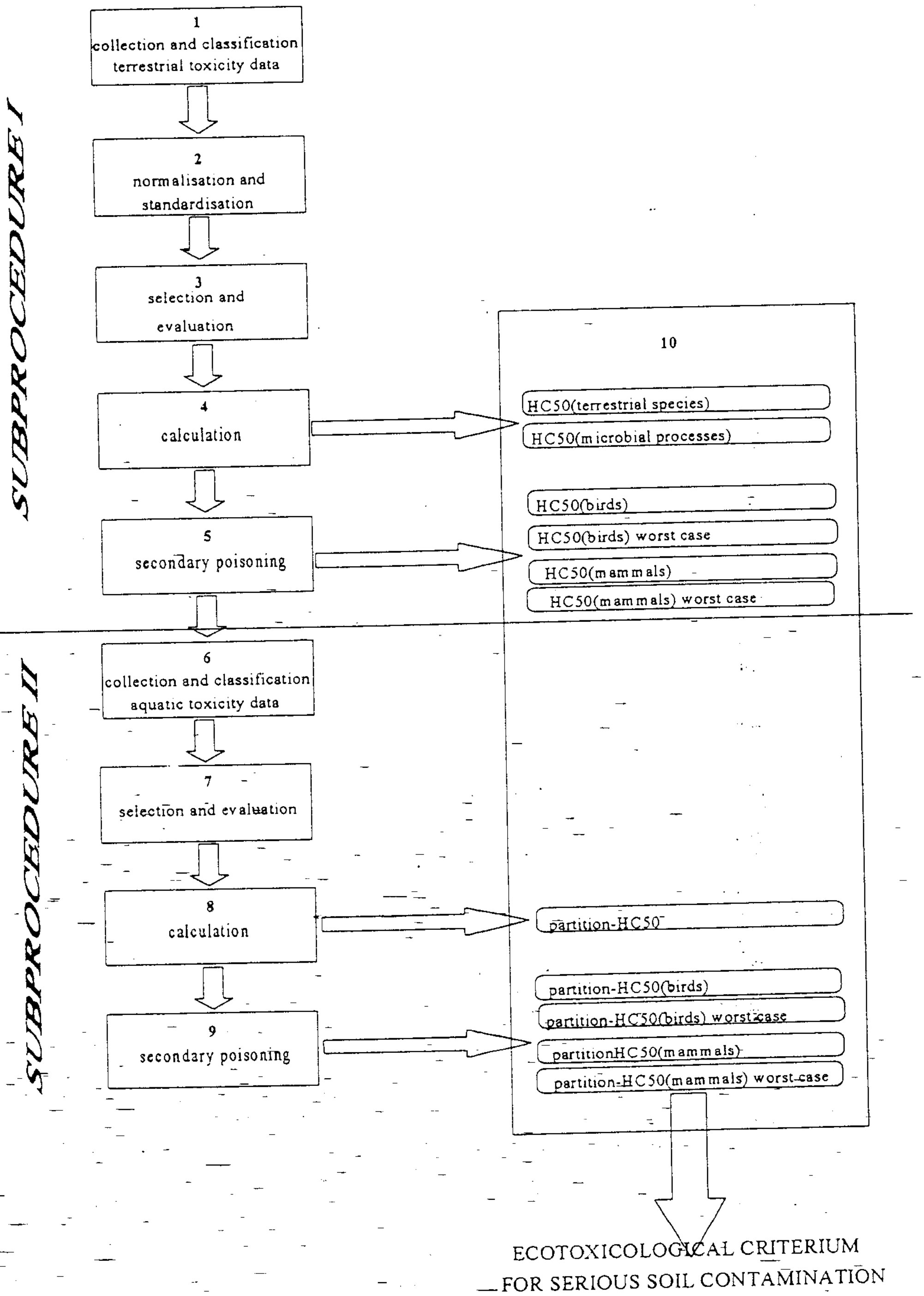

Figure 1: Schematic presentation of the protocol used to derive ecotoxicological criteria for serious soil contamination.

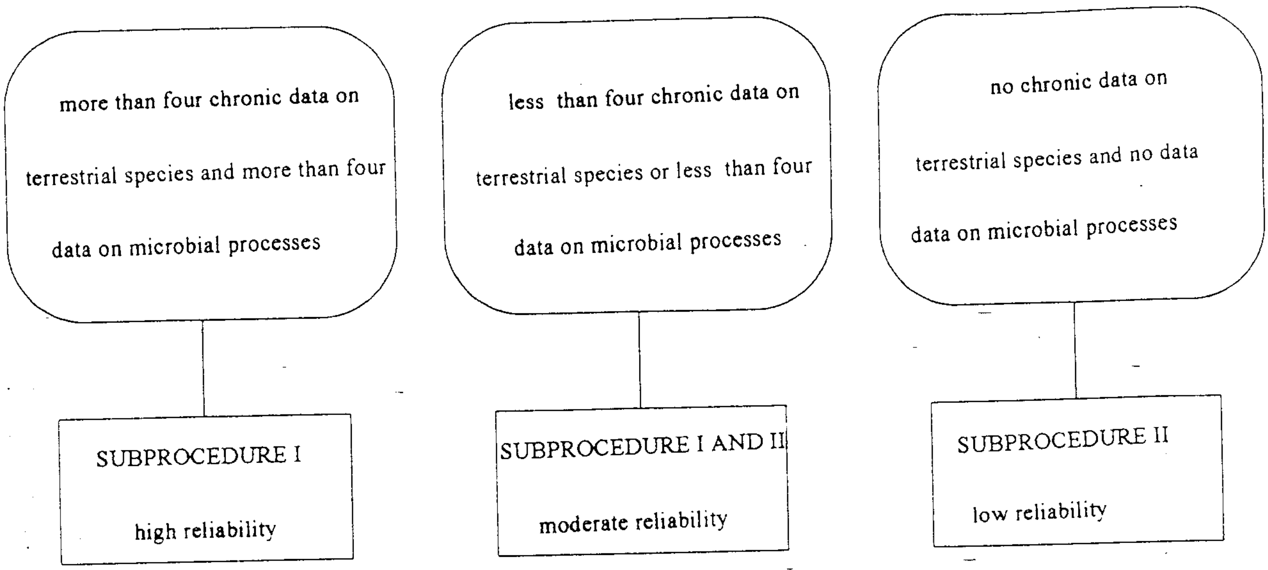

Figure 2: Subprocedures used and reliability of ecotoxicological criteria for serious soil contamination.

3. PROTOCOL FOR THE DERIVATION OF ECOTOXICOLOGICAL CRITERIA FOR SERIOUS SOIL CONTAMINATION

3.1. COLLECTION AND CLASSIFICATION OF TERRESTRIAL DATA

*Collect data on the toxicity of the substance for terrestrial species, microbial processes and enzymatic activity. Classify the data found for terrestrial species (raw data IA) and microbial processes and enzymatic activity (raw data IB) separately in 1: chronic toxicity data and
2: acute toxicity data.
Report the species or process studied, the criterion considered (NOEC or L(E)Cx) and result in mg/kg dry soil, together with the experimental conditions; parameters as soil type, test-substance purity, pH, organic matter- and clay content of the soil, temperature and exposure time are necessary.

*If $\log K_{ow} > 5$ and $MW < 600$, or when the substance is a metal for which secondary poisoning is to be expected, collect also NOECs and L(E)Cx's for birds and mammals and BCFs for worms.

-Classify data for birds (raw data IIA) and mammals (raw data IIB) separately in
1: chronic toxicity data and
2: acute toxicity data.
Report the species studied, the criterion considered (NOEC or L(E)Cx) and result in mg/kg bodyweight or mg/kg food, together with the experimental conditions; parameters as age or size of the species used, test-substance purity and exposure route are necessary.

Classify data on BCFs (raw data IIC) for each worm species separately. Report the species studied and result together with the experimental conditions; parameters as soil type, test-substance purity, pH, organic matter- and clay content, temperature and exposure time are necessary. When no experimental data on worms are available, for lipophilic compounds, a BCF worm can be estimated using the K_{ow}. Calculate BCF as follows:

$$worm : BCF = 0.0257\ K_{ow}^{0.07}$$

BOX 3.1.1. DATA NEEDED FOR THE DERIVATION OF ECOTOXICOLOGICAL CRITERIA FOR SERIOUS SOIL CONTAMINATION

The aim of the ecotoxicological criterium for serious soil contamination is to protect at least 50% of all the species and microbial processes in a terrestrial ecosystem. For this aim a statistical extrapolation method is used, based on the effects through direct exposure of single species and microbial processes (BOX 3.4.1.).

Parameters like reproduction, growth and survival are considered to be essential for the criterium for the protection of species (Slooff, 1992). This means that there is a serious danger when a substance is present in a concentration exceeding the No Observed Effect Concentration of one of those parameters for 50% of the species. Toxicity data on single species are used to estimate the concentration for protection of species.

Besides this, effect parameters for microbial processes have to be regarded separately (TCB, 1992). There is a serious danger for microbial processes when a substance is present in a concentration exceeding the No Observed Effect Concentration for 50% of the microbial processes and enzymatic activity. Toxicity data on microbial process, like e.g. denitrification and various enzyme activities are used to asses the 50 % level for protection of microbial processes.

For some substances, (top)predators may be endangered by exposure to contaminated food, through the mechanism of secondary poisoning. Methods for risk assessment on secondary poisoning, through ingestion of contaminated food were developed (BOX 3.5.1.). To incorporate secondary poisoning, data on the toxicity of the substance for birds and mammals and bioconcentration factors (BCFs) for worms are used. For the derivation of reliable BCFs preference is given to the use of experimentally derived BCFs over QSAR estimates. When no experimental data on BCFs are available QSAR estimates are used (BOX 3.1.3).

BOX 3.1.2. COLLECTION OF RELIABLE DATA

Not all data found in the literature can be used. Data should be reliable and give an unambiguous value for a NOEC, L(E)C50, BCF or K_{ow}. A study is considered to be reliable if the design of the experiment is in agreement with international accepted guidelines such as the OECD guidelines (OECD). To judge studies which have not been performed according to these guidelines, criteria are developped at the Toxicology Advisory Centre (ACT, 1994). These procedures, together with expert judgement of the person performing the data collection, are necessary to derive reliable sets of raw data.

As was mentioned before parameters like reproduction, growth and survival are considered to be essential for the criterium for protection of species (BOX 3.1.1, Slooff, 1992). To evaluate the impact of long term exposure to low concentrations of a substance, especially long term tests are of importance.

Toxicity-tests are divided in acute- (short-term) and chronic (long-term) tests. The definitions for acute and chronic are derived from ECETOC (1994): acute exposure of animals covers any period up to one third of the time taken from "birth" to sexual maturity. Any more lengthy exposure, is defined as chronic. This means that the definition of acute and chronic depends on the life-expectancy of a species.

Tests with aquatic species are abundant and for the decision if a test must be categorised acute or chronic, it is referred to these guidelines (OECD). Tests with terrestrial species are however scarce. The decision if a terrestrial test should be categorised acute or chronic should be evaluated case by case on the basis of ecological information of the species.

BOX 3.1.3. CALCULATION OF BCFs FOR WORMS WHEN NO EXPERIMENTAL DATA ARE AVAILABLE (Romijn et al., 1991b)

For organic chemicals a QSAR is reported by Connell and Markwell (1990) in which BCF can be estimated using K_{ow}:

$$BCF = (Y_l/(x*f_{oc}) *K_{ow}^{b-a}$$

in which:

Y_l = the lipid fraction of earthworms

x = a constant, estimate to be 0.66 by Rao and Davidson (1980)

f_{oc} = the organic carbon fraction of the soil. The organic carbon content of a soil can be calculated from the organic matter content by dividing through 1.7. Since values for organic compounds will be standardised for a 10% OM soil, %OC can be set equal to 5.9

K_{ow} = the octanol-water partition coefficient

b-a = b and a are both non linearity constants, a for the soil to soil-water partitioning and b for the soil-water to earthworm partitioning. b-a was estimated by Markwell et al. (1989) to equal 0.07 for earthworms.

This formula (when b-a=0.07) shows that BCFs for worms are only weakly dependent on the K_{ow}. The Lipid content of the worm (Y_l) and the organic carbon fraction in the soil (f_{oc}) determine the BCF. Rao and Davidson (1980) report an average lipid content of 0.84%. Belfroid et al. (1991) found values ranging from 0.63% to 2%. For calculation of BCFs Romijn et al. (1991b) used a lipid content of 1%.

When assuming a lipid content of 1% the formula can be rewritten as follows:

$$BCF = 0.0257\ K_{ow}^{0.07}$$

3.2. NORMALISATION AND STANDARDISATION OF COLLECTED TERRESTRIAL DATA

*The data for terrestrial species (raw data IA) and for microbial processes (raw data IB) of organic chemicals have to be normalised to a standard soil (OM=10, L=25) using the following equation:

$$NOEC_{standard} ; LC50_{standard} = NOEC_{experiment} ; LC50_{experiment} \frac{OM_{standard}}{OM_{experiment}}$$

When OM<2, use OM=2 and for OM>30 use OM=30 in the calculations.

*The data for terrestrial species (raw data IA) and for microbial processes (raw data IB) of metals have to be normalised to a standard soil (OM=10, L=25) using the following equation:

$$NOEC_{standard} ; LC50_{standard} = NOEC_{experiment} ; LC50_{experiment} \frac{R(L;OM)_{standard}}{R(L;OM)_{experiment}}$$

R values for different soil compositions can be derived from formulas defined on the basis of background values of metals found in the Netherlands (VROM, 1990; De Bruijn and Denneman, 1992).

*BCF-values for worms (raw data IIC) have to be recalculated for experimental conditions using the following criteria:
-Experimentally derived BCFs have to be reported for whole body of worm, express BCFs in mg substance/kg wet weight worm divided by mg substance/dry weight of soil.
-20% humidity is used as standard to transform data on concentrations in soil expressed as mg/kg wet weight to a mg/kg dry weight.
-wet weight=5*dry weight is used as a standard for transforming data on concentrations in worms given as mg/kg dry weight into mg/kg wet weight, unless the actual ratio is mentioned in the study.

*BCF values for organic chemicals have to be normalised to a standard soil (OM=10, L=25) using the following equation:

$$BCF_{standard} = BCF_{experiment} \frac{OM_{standard}}{OM_{experiment}}$$

BOX 3.2.1. NORMALISATION AND CORRECTION OF TERRESTRIAL DATA

The toxicity of a substance varies depending on the soil characteristics due to differences in bioavailability of the substance. Data found in the literature are often deduced from experiments with different experimental conditions. Denneman and van Gestel (1990) proposed to normalise toxicity data for terrestrial species and microbial processes to a standard soil, consisting of 10% organic matter (OM) and 25% clay (L).

For organic substances the bioavailability is particulary determined by the organic matter content (van Gestel and Ma, 1988; 1990) For metals however more than one soil property determine bioavailability, exact descriptive formulas are not available. Normalisation of toxicity data is based on background concentrations found in the Netherlands (VROM, 1990; De Bruijn and Denneman, 1992).

BCF values for worms show a large variation due to factors causing differences in bioavailability (Romijn et al., 1991b). When possible BCF data have to be standardised and normalised to a standard soil in order to reduce variability. Connell and Markwell (1990) found a strong correlation between BCF and %OM for a large set of organic chemicals. This correlation was confirmed by results of a regression analysis for dieldrin and DDT by Romijn et al. (1991b). For metals it is yet not possible to decide which soil parameter shows the highest correlation with BCFs. It has to be decided on the information available if normalisation is possible.

3.3. SELECTION AND EVALUATION OF TERRESTRIAL DATA

*Select toxicity data for terrestrial species (selected data IA) and for microbial processes (selected data IB) to be used in the calculation of HC50s taking into account the following criteria (Slooff, 1992):
-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.
-If for one test species several toxicity data are available based on different toxicological endpoints, only the lowest value is used.
-When for one species the same parameter is determined at different temperatures, select the one which is performed at the most realistic temperature.

*If less than 4 toxicity data from different taxonomic groups are available after selection, collect also aquatic toxicity data (step 6 of the protocol).

*If data on the toxicity for birds, mammals and BCFs are collected: select toxicity data for birds (selected data IIA), mammals (selected data IIB) and BCFs for worms (selected data IIC) to be used in the calculation of HC50s taking into account the same criteria as mentioned above for the toxicity data on terrestrial species and microbial processes (Slooff, 1992).

BOX 3.3.1. AVAILABILITY OF DATA
The outcome of statistical extrapolation methods will be more reliable when more data are available. To reduce the uncertainty of the estimated median sensitivity and to meet the species variety of an ecosystem to some extent, the limitation is set that at least four chronic NOECs of different taxonomic groups should be available (Okkerman et al., 1992). When less data are available, also data on the toxicity of the compound for aquatic organisms are necessary (BOX 3.8.1.).

BOX 3.3.2. TAXONOMIC GROUPS

Effects of toxic substances are determined by the amount present in the organism, which depends on characteristics of the species, environmental conditions and the characteristics of the substance itself. Species-specific processes determining the accumulating potential are uptake, excretion and internal storage, which are related to the anatomical and physiological design of an organism.

Within a soil ecosystem a variety of groups of species are represented (Dindal, 1989; Swift et al., 1979). Between closely related species toxicological relationships are to be expected based on similarities in anatomical and physiological design of the species. This possible relationship has to be kept in mind when using data in statistical extrapolation methods.

Classifying soil organisms into groups on the basis of anatomical and physiological design does not completely follow the taxonomic classification. The proposed groups are shown below. This selection is based on toxicological information available at present. As mentioned before data on sensitivity of soil species is scarce compared to data availability in aquatic ecotoxicology. Therefore this classification can be used until further data ask for an adapted-classification.

Selected groups

Bacteria
Protozoa
Macrophyta
Fungi
Platyhelminthes
Nematoda
Gastropoda
Annelida
Arachnida
Insecta
Diplopoda
Chilopoda
Isopoda

The taxonomic hierarchy is given in Appendix II as background information.

3.4. CALCULATION OF HC50(terrestrial species) AND HC50(microbial processes)

*For selected data for terrestrial species (IA) and microbial processes (IB) separately
-1: Calculate the geometric mean of all the NOECs
-2: Calculate the geometric mean of the L(E)C50s. Divide this geometric mean by 10
-3: Calculate the geometric mean of the outcome of 1 and 2

BOX 3.4.1. STATISTICAL EXTRAPOLATION METHOD

The statistical extrapolation method used for derivation of environmental quality criteria in the Netherlands, is based on the assumption that the sensitivities of species in an ecosystem can be described by a statistical frequency distribution. For a detailed overview of the theory and the statistical adjustments since its introduction, one is referred to the original literature (Kooijman, 1987; van Straalen and Denneman, 1989; Aldenberg and Slob, 1993; Wagner and Lokke, 1991).

For the derivation of ecotoxicological criteria for serious soil contamination, the method described by Aldenberg and Slob (1993) is used. The protection level of the ecotoxicological criterium for serious soil contamination is set on a level that protects 50% of all the species and microbial processes in an ecosystem (BOX 3.1.1). To ensure that both species and microbial processes are protected a HC50 for both is derived independently. This means that there is a serious danger when a substance is present in a concentration exceeding the No Observed Effect Concentration for 50% of the species and exceeding the No Observed Effect Concentration for 50% of the microbial processes.

Estimation of this 50% levels of the assumed statistical distributions is reduced to calculating the geometric mean of the data available. Chronic data are most important (BOX 3.1.2.). Acute toxicity data are divided with a application factor 10 to adjust for the short duration of the experiments.

3.5. SECONDARY POISONING

*If there is a potential risk for secondary poisoning and data on the toxicity of the compound for birds and mammals and BCFs for worms have been selected (see step 1 of the protocol) secondary poisoning-HC50s have to be derived.

*For selected data for birds (IIA), mammals (IIB) and BCFs (IIC):
-1: Calculate the geometric mean of the BCFs
-2: Calculate the geometric mean of all the NOECs for birds and mammals separately.
-3: Calculate the geometric mean of the L(E)C50s. Divide this geometric mean by 100 fore birds and mammals separately.
-4: Calculate the geometric mean of the outcome of 2 and 3 for birds and mammals separately. These values are the HC50(birds) and HC50(mammals) expressed in a concentration in the (laboratory)food.
-5: Recalculate the outcomes of 4 to a corrected concentration in the soil, by using the following equation:

$$HC50_{birds}\ ;\ HC50_{mammals} = \frac{HC50_{birds}\ ;\ HC50_{mammals} * 0.23}{BCF_{worm}}$$

BOX 3.5.1. HOW TO INCLUDE SECONDARY POISONING

Several models have been developed for estimating the risk for secondary poisoning (van der Weiden and de Bruijn, 1994). At this moment the algorithms developed by Romijn et al. (1991a; 1991b) are used in the derivation of quality objectives in the Netherlands. Romijn et al. (1991a; 1991b) analyzed two simple food chains. An algorithm was proposed to calculate effect concentrations for secondary poisoning by dividing toxicity data based on food intake by the BCF to a concentration in the soil or water. In addition proposals have been made for refining the methods by taking into account energy-requirements and differences in diet between laboratory animals and field animals (BOX 3.5.2.).

When using the algorithms developed by Romijn et al. (1991a; 1991b) two methods can be applied to incorporate the risk for secondary poisoning in the derivation of ecotoxicological criteria for serious soil contamination: First, two independent effect concentrations can be derived, one for species exposed through the soil and one for species exposed through food (birds and mammals). Second, all data for terrestrial species and data for birds and mammals can be lumped and used for the calculation of one effect concentration.

For the derivation of ecotoxicological criteria for serious soil contamination the first method is chosen because it is questionable if the 50% criterium protects both species exposed directly through the soil and species exposed through the food. More related species are expected to have a more related sensitivity and by deriving one value (method 2), there is a risk that all birds or/and mammals are within the unprotected 50% of species.

It is recognised that the methods developed can be regarded as a pragmatic approach for obtaining a rough initial indication of the potential for secondary poisoning. In view of the major uncertainties and the limited number of (simple) foodchains considered, extensive follow-up research will be required (concerning detailed local-specific and species-specific information, when a substance with a potential for secondary poisoning is found (Health Council of the Netherlands, 1993).

BOX 3.5.2. CORRECTION AND RECALCULATION OF HC50(birds) AND HC50(mammals)

Toxicity data for birds and mammals are derived from toxicity studies in the laboratory. The experimental conditions are far from realistic compared to the field conditions. In the first place the food used in the laboratory is different from food eaten in the field. In the second place, the metabolic requirements are not similar under laboratory and field condition. To adjust for these differences correction factors have been derived for the different foodtypes used (Everts et al. 1992). The HC50(birds) and HC50(mammals) have to be corrected for these differences.

Ecotoxicological effect concentrations for terrestrial species and microbial processes are based on concentrations in soil, or in the case of aquatic species on a concentration in the water. For birds and mammals however, effect concentrations are expressed in a concentration in the food. The HC50(birds) and HC50(mammals) have to be recalculated to a concentration in the soil or water to make it possible to compare the different HC50s with each other.

Recalculation is done by dividing the HC50(birds) and HC50(mammals) by the BCF for worms of the substance regarded. When deriving aquatic HC50s BCFs for fish and mussels are used. In all cases, worm, fish or mussel, besides the geometric mean of the BCFs also the highest BCF is used, to check for a worst case.

3.6. COLLECTION AND CLASSIFICATION OF AQUATIC DATA

*Collect data on the toxicity of the substance for freshwater and marine species. Classify the data found for freshwater species (raw data IIIA) and marine species (raw data IIIB) separately in

1: chronic toxicity data and
2: acute toxicity data.

Report the species, the criterion considered (NOEC or L(E)Cx) and result in mg/l or µg/l together with the experimental conditions; parameters as test-type, test-substance purity, pH, hardness in the case of freshwater species or salinity in the case of marine species, temperature and exposure time are necessary.

*When less than 4 chronic toxicity data are available, and the substance in question can be classified as an inert chemical (acting by polar narcosis) with no specific mode of action, QSAR derived NOECs may be derived and added to the raw data.

*If $\log K_{ow} > 5$ and $MW < 600$, or when the substance is a metal for which is to be expected, collect also NOECs and L(E)Cx's for birds and mammals and BCFs for fish and mussels.

Classify data for birds (raw data IIA) and mammals (raw data IIB) separately in

1: chronic toxicity data and
2: acute toxicity data.

Report the species studied, the criterion considered (NOEC or L(E)Cx) and result in mg/kg bodyweight or mg/kg food, together with the experimental conditions; parameters as age or size of the species used, test-substance purity and exposure route are necessary.

Classify data on BCFs for each mussel- and fish species separately (raw data IID, fish and IIE, mussels). Report the species studied and the value of the BCF based on wet weight, together with the experimental conditions; parameters as test-type, test-substance purity, test water, pH, hardness, temperature and exposure time are necessary.

*When no experimental data on BCF for fish and mussels are available, for lipophilic compounds, a BCF can be estimated using the K_{ow}. Calculate BCF as follows:

$$fish\ ;\ mussel:\ BCF = 0.048\ K_{ow}$$

*Collect data on the sorption of the substance to soil (raw data IV). Report the logKoc together with the experimental conditions like soil type used, % organic carbon, pH, CEC, solid/water ratio and equilibrium time used in the experiment. When no experimental data on the sorption are available log Koc can be calculated using an Kow.

BOX 3.6.1. DATA NEEDED FOR THE DERIVATION OF HC50-VALUES THROUGH EQUILIBRIUM PARTITION

When insufficient terrestrial data are available, HC50-values can be derived by applying the equilibrium partition method using data on the sensitivity of aquatic species (BOX 3.8.1.). When applying this method, toxicity data on single species (freshwater and marine) are used to estimate a HC50(aquatic species).

As for terrestrial species, there is a serious danger for species when a substance is present in a concentration exceeding the No Observed Effect Concentration for 50% of the species. For some substances, toppredators may be endangered by exposure to contaminated food, through the mechanism of secondary poisoning (BOX 3.5.1). To incorporate secondary poisoning, data on the toxicity of the substance for birds and mammals and bioconcentration factors for fish and mussel are necessary. (BOX 3.6.4.).

The equilibrium partition method (EP method) (BOX 3.8.1.) is used to derive a soil water concentration from the concentration in the total soil. Therefore data on the sorption of the substance are needed. The soil -water partition coefficients (K_p) describe the equilibrium distribution of a chemical over a solid phase (soil, sediment or suspended matter) and water. $K_p = C_{water}/ C_{soil}$ in l/kg where C_{water}= equilibrium concentration in water (mg/dm^3) and C_{soil} = equilibrium concentration in soil (mg/kg).

BOX 3.6.2. SENSITIVITY OF FRESHWATER- AND MARINE SPECIES

So far there are no indications that freshwater species are more or less sensitive than marine species. For some substances however, differences may be expected as a result of differences in bioavailability of a substance. Therefore data have to be reviewed critically before using these in the statistical extrapolation method. Freshwater and marine toxicity data are combined unless analysis of the data indicates a different sensitivity (RWS, 1992)

BOX 3.6.3. QSAR DERIVED NOECs

Experimentally derived NOECs for aquatic species are preferred when deriving ecotoxicological criterium through equilibrium partition. If the chemical can be classified as an inert chemical (which means that the substance is acting by narcosis), and with no specific mode of action, reliable Q(uantitative) S(tructure)-A(ctivity) R(elationship) equations for a number of test species are available, to derive chronic NOECs (van Leeuwen et al., 1992). These QSAR derived NOECs can be used, when only few experimental toxicity data are available. In order to determine if a substance is acting by narcosis a classification scheme developed by Verhaar et al. (1992) can be used.

BOX 3.6.4. CALCULATION OF BCFs FOR FISH AND MUSSEL WHEN NO EXPERIMENTAL DATA ARE AVAILABLE

Contrary to BCFs for worm, BCFs for fish and mussel are mainly substance dependent. For organic chemicals a QSAR is reported by Mackay (1982) in which BCF can be estimated using Kow:

$$BCF = 0.048\ K_{ow}$$

BOX 3.6.5. CALCULATION OF Kp WHEN NO EXPERIMENTAL DATA ARE AVAILABLE

Experimentally derived Kp's are preferred. Kp-values from the literature are calculated to an organic carbon normalised partition coefficient Koc: Koc= Kp/f_{oc} in which f_{oc} is the fraction organic carbon of the soil used in the experiment (Bockting et al., 1993). Afterwards these Koc-values can be calculated to an Kp for a standard soil in which f_{oc} = 0.059. When no experimental data are available Kp's can be calculated using K_{ow}'s. For this aim several regression equations exist; for a detailed overview one is referred to the original literature (Karickhoff, 1981; DiToro et al., 1991 and Gerstl, 1990).

3.7. SELECTION AND EVALUATION OF AQUATIC DATA

*Select toxicity data for freshwater species (raw data IIIA) and for marine (raw data IIIB), birds (raw data IIA), mammals (raw data IIB) and BCFs for fish and mussels (raw data IID and IIE) to be used in the calculation of HC50s taking into account the following criteria (Slooff, 1992):

-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.

-If for one test species several toxicity data are available based on different toxicological endpoints, only the lowest value is used.

-When for one species the same parameter is determined at different temperatures, select the one which is performed at the most realistic temperature.

*If less than 4 toxicity data from different taxonomic groups are available after selection, it is not possible to derive a partition-HC50.

BOX 3.7.1. AVAILABILITY OF DATA

The outcome of statistical extrapolation methods will be more reliable when more data are available. To reduce the uncertainty of the estimate of the median sensitivity made and to meet the species composition of an ecosystem to some extent, the limitation is set that at least four chronic NOECs of different taxonomic groups should be available (Okkerman et al., 1992). When less data are available, it is not possible to calculate a partition-HC50.

BOX 3.7.2. TAXONOMIC GROUPS (SEE ALSO BOX 3.3.2..)

A division of aquatic species into groups on the basis of anatomical and physiological design does not completely follow the taxonomic classification. The proposed groups are shown below. This selection of groups to be used as "taxonomic groups" is based on toxicological information available at present.

Selected groups

Bacteria
Cyanophyta
Protozoa
Algae (can be subdivided into Chrysophyta, Euglenophyta, Dinophyta, Cryptophyta, Chlorophyta)
Macrophyta
Coelenterata
Platyhelminthes
Nematoda
Mollusca
Annelida
Insecta
Crustacea
Pisces
Amphibia
Echinodermata

The taxonomic hierarchy is given in Appendix II as background information.

3.8. CALCULATION OF HC50(aquatic organisms) AND partition-HC50.

*For selected data for aquatic freshwater species (IIIA) and marine species (IIIB):
-1: Calculate the geometric mean of all the NOECs.
-2: Calculate the geometric mean of the L(E)C50s. Divide this geometric mean by 10.
-3: Calculate the geometric mean of 1 and 2. This value is the HC50 (aquatic organisms).
-4: Calculate the partition-HC50 using the following equation:

$$\text{partition-HC50} = K_p * \text{HC50(aquatic organisms)}$$

BOX 3.8.1. THE EQUILIBRIUM PARTITION METHOD

The equilibrium partition method (EP method) was originally proposed by Pavlou and Weston (1984) to develop sediment quality criteria. The concept has been described in detail by Shea (1988) and DiToro et al. (1991). The method models the tendency of a chemical to move from one environmental compartment to another. Soil-water partition coefficients (Kp) describe the equilibrium distribution of a chemical over a solid phase (soil, sediment or suspended matter) and water.

When not sufficient data for terrestrial organisms are available this method can be used to calculate a concentration in the soil from a concentration in the water. Two important assumptions are made when applying this method: First it is assumed that uptake of substances is mainly through the porewater; second it is assumed that the sensitivity of terrestrial and aquatic species is comparable.

3.9. SECONDARY POISONING

*For selected data for birds (IIA), mammals (IIB) and BCFs for fish (IID) and mussels (IIE)
-1: Calculate the geometric mean of the BCFs for fish and mussels separately
-2: Calculate the geometric mean of all the NOECs for birds and mammals separately.
-3: Calculate the geometric mean of the L(E)C50s for birds and mammals separately. Divide this geometric means by.
-4: Calculate the geometric mean of the outcome of 2 and 3 for birds and mammals separately. These values are the HC50(birds) and HC50(mammals) expressed in a concentration in the (laboratory)food.
-5: Recalculate the outcomes of 4 to a concentration in the water, using the following equations:

$$fish: HC50_{(birds)} ; HC50_{(mammals)} = \frac{HC50_{(birds)} ; HC50_{(mammals)} * 0.32}{BCF_{fish}}$$

$$mussel: HC50_{(birds)} ; HC50_{(mammals)} = \frac{HC50_{(birds)} ; HC50_{(mammals)} * 0.20}{BCF_{mussel}}$$

-6: Recalculate the outcome of 5 into a concentration in soil using the following equation:

$$partition\text{-}HC50(birds;mammals) = Ksubp * HC50(birds;mammals)$$

BOX 3.9.1. HOW TO INCLUDE SECONDARY POISONING = BOX 3.5.1.

BOX 3.9.2. RECALCULATION AND CORRECTION OF HC50(birds) AND HC50(mammals) =BOX 3.5.2.

3.10. DERIVING THE ECOTOXICOLOGICAL CRITERIUM FOR SERIOUS SOIL CONTAMINATION

*Collect the separately derived values:

- HC50(terrestrial species) from step 4
- HC50(microbial processes) from step 4
- HC50(birds) from step 5
- HC50(birds; worst case) from step 5
- HC50(mammals) from step 5
- HC50(mammals; worst case) from step 5

-partition-HC50 from step 8
-partition-HC50(birds) from step 9
-partition-HC50(birds; worst case) from step 9
-partition-HC50(mammals) from step 9
-partition-HC50(mammals; worst-case) from step 9

*Derive an ecological criterium for serious soil contamination from these values

BOX 3.10.1 RELIABILITY OF VALUES

Criteria for serious soil contamination have to be derived from the information available. It has to be kept in mind that depending on the amount of data available the separate values are more or less reliable. Especially in this step, it is necessary to judge the reliability of the separate values by expert judgement.

-When both the HC50(terrestrial species) and HC50(microbial processes) are based on more than 4 toxicity data, the lowest is selected as a reliable criterium for serious soil contamination.
-When also a partition-HC50 is derived, the derivation of the criterium for serious soil contamination has to be judged on the basis of toxicity data and sorption data available, case by case. The criterium for serious soil contamination is noted as moderate reliable.
-When only a partition-HC50 can be derived the criterium for serious soil contamination is noted as not reliable.
-The values for secondary poisoning are used as a check to evaluate if there is a risk for secondary poisoning. When there is a risk for secondary poisoning, which means that the (partition-)HC50(birds) and HC50(mammals) are lower than the HC50(terrestrial species) and HC50(microbial processes), the criterium for serious soil contamination has to be adjusted.

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APPENDIX I: List of HC50-definitions

- **HC50(terrestrial species)**: HC50 using toxicity data on terrestrial species as input; estimated median sensitivity of terrestrial species in mg/kg soil.
- **HC50(microbial processes)**: HC50 using toxicity data on microbial processes and enzymatic acticity as input; estimated median sensitivity of microbial processes in mg/kg soil.
- **HC50(birds)**: HC50 using toxicity data on birds as input; Recalculated median sensitivity of birds in mg/kg soil using the mean BCF for worms
- **HC50(birds; worst case)**: HC50 using toxicity data on birds as input; Recalculated median sensitivity of birds expressed in mg/kg soil using the highest BCF for worms, indicating a worst case situation.
- **HC50(mammals)**: HC50 using toxicity data on mammals as input; Recalculated median sensitivity of birds expressed in mg/kg soil using the mean BCF for worms
- **HC50(mammals; worst case)**: HC50 using toxicity data on mammals as input; Recalculated median sensitivity of birds expressed in mg/kg soil using the highest BCF for worms, indicating a worst case situation.

- **HC50(aquatic species)**: HC50 using toxicity data on aquatic species as input; estimated median sensitivity of aquatic species in mg/l.
- **partition-HC50**: Through equilibrium partition method derived median sensitivity of terrestrial species in mg/kg soil
- **partition-HC50(birds)**: Through equilibrium partition method derived recalculated median sensitivity of birds expressed in mg/kg soil using the mean BCF for fish or mussel.
- **partition-HC50(birds; worst case)**: Through equilibrium partition method derived and recalculated median sensitivity of birds expressed in mg/kg soil using the highest BCF for fish or mussel, indicating a worst case situation.
- **partition-HC50(mammals)**: Through equilibrium partition method derived recalculated median sensitivity of mammals expressed in mg/kg soil using the mean BCF for fish or mussel.
- **partition-HC50(mammals; worst case)**: Through equilibrium partition method derived and recalculated median sensitivity of mammals expressed in mg/kg soil using the highest BCF for fish or mussel, indicating a worst case situation.

APPENDIX II: Taxonomical position of selected groups (terrestrial species)

REGNUM	phylum	sub phylum	class	sub class	order	sub order	family
MONERA							
	Bacteria						
	Cyanophyta						
PROTISTA							
	protozoa						
	algae						
	Ciliophora						
	Sarcodina						
	mastigophora						
MACROPHYTA							
FUNGI							
ANIMALIA							
	Platyhelminthes		Turbellaria				
	Nematoda		Secernentea				
			Adenophorea				
	Mollusca		Gastropoda	Prosobranchia			
				Pulmonata			
	Annelida		Oligochaeta		Tubificida	Enchytraeina	Enchytraeidae
					Haplotaxida	Lumbricina	Lumbricidae
							Megascolocidae
	Tardigrada						
	Arthropoda	Chelicerata	Arachnida		Pseudo-scorpionida		
					Opiliones		
					Acarina		
					Araneida		
		Uniramia	Insecta	Apterygota	Diplura		
					Protura		
					Thysanura		
					Collembola		
				Pterygota	Ephemeroptera		
					Odonata		
					Orthoptera		
					Isoptera		
					Plecoptera		
					Dermaptera		
					Embioptera		
					Psocoptera		
					Zoraptera		
					Mallophaga		
					Anoplura		
					Thysanoptera		
					Hemiptera		
					Homoptera		
					Neuroptera		
					Coleoptera		
					Strepsiptera		
					Mecoptera		
					Trichoptera		
					Lepidoptera		
					Diptera		
					Hymenoptera		
					Siphonaptera		
			Diplopoda				
			Pauropoda				
			Symphyla				
			Chilopoda				
		Crustacea	Malacostraca	Eumalastraca	Isopoda		

APPENDIX III: Taxonomical position of selected groups (aquatic species)

REGNUM	phylum	sub phylum	super class	class	sub class	order	sub order
MONERA							
	Bacteria						
	Cyanophyta						
PROTISTA							
	Protozoa						
	Algae						
	Mastighophora						
	Ciliophora						
	Sarcodina						
	Chiliophora						
MACROPHYTA							
ANIMALIA							
	Porifera						
	Coelenterata			Hydrozoa			
				Scyphozoa			
				Anthozoa			
	Ctenophora			Tentaculata			
				Nuda			
	Platyhelminthes			Turbellaria			
	Nematoda						
	Gastrotricha						
	Rotifera						
	Mollusca			Gastropoda			
				Bivalvia			
				Scaphopoda			
				Cephalopoda			
	Annelida			Polychaeta			
				Oligochaeta			
				Hirudinae			
	Arthropoda	Chelicerata		Pycnogonida			
				Arachnida		Acarina	
		Crustacea		Branchiopoda			
				Ostracoda			
				Mystacocarida			
				Copepoda			
				Branchiura			
				Cirripedia			
				Malocostraca			
		Uniramia		Insecta	Apterygota		
					Pterygota	Ephemeroptera	
						Odonata	
						Trichoptera	
						Diptera	
	Echinodermata		Stelleroidea				
				Echinoidea			
				Holothuroidea			
				Crinoidea			
	Chordata	Hemichordata					
		Urochordata					
		Cephalo-chordata					
		Vertebrata	Pisces				
			Tetrapoda	Amphibia			
				Reptilia			
				Aves			
				Mammalia			