NATIONAL INSTITUTE OF
PUBLIC HEALTH AND THE ENVIRONMENT
BILTHOVEN, THE NETHERLANDS

RIVM report 601506 001

Protocol for derivation of Harmonised Maximum Permissible Concentrations (MPCs)

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March 1999

This research was carried out by order and for the account of the Directorate General for Environmental Protection, Directorate for Chemicals, External Safety and Radiation Protection and Directorate for Water and Agriculture, in the framework of the projects: Setting integrated environmental quality standards (project no. 601501) and Consultancy on risk assessment for pesticides (project no. 601506).

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ABSTRACT

In this report a procedure is described for deriving harmonised Maximum Permissible Concentrations (MPCs). This procedure is developed because different MPCs are operative in the frameworks 'Setting of Integrated Environmental Quality Standards', registration of plant protection products and of biocides and it is undesirable that two or three different MPCs for the same compound coexist.

A search profile for literature is presented. Reliability criteria will be used to evaluate the studies (public literature and confidential reports) underlying the MPC derivation. The selection of ecotoxicological endpoints for MPC derivation depends on the amount, reliability and the kind of data.

Two methods will be used to derive harmonised MPCs from ecotoxicological studies (direct methods and indirect methods). Direct methods: the refined effect assessment method (Aldenberg and Slob, 1993) and the preliminary effect assessment method (TGD (ECB, 1996)). Which of the methods is applied depends on the data availability. MPCs for soil and sediment can also be derived indirectly from the MPC water with the equilibrium partitioning method (Ep-method), if experimental data are lacking. The latter method will also be used to harmonise the MPCs for the individual environmental compartments. The possible potential risk for secondary poisoning will be assessed if compounds have a log $K_{ow} > 5.0$ and/or have low depuration or high accumulation rates. This means that MPCs in lower compartments will be adjusted based on the accumulation potential of a compound in top predators.

CONTENTS

SAMENVATTING

In Nederland is het op dit moment mogelijk dat in het kader van Integrale Normstelling (INS) een andere MTR waarde is afgeleid dan in het kader voor de toelating van bestrijdingsmiddelen en biociden voor eenzelfde stof. Omdat dit een onwenselijke situatie is, is besloten de verschillende procedures voor het afleiden van MTRs te harmoniseren.

MTR waarden voor bestrijdingsmiddelen zullen worden afgeleid op het moment dat het produkt wordt aangemeld voor (her)registratie. Afleiding vindt ook plaats indien de 'tenzij' bepalingen in de bestrijdingsmiddelenwet niet van toepassing zijn.

Een zoekprofiel voor literatuur is opgesteld. Voor de evaluatie van de studies die gebruikt worden voor afleiding van de MTRs is gebruik gemaakt van Mensink *et al.* (1995) en Kalf (1996). De genoemde evaluatie methoden zullen voor zowel de vertrouwelijke rapporten als de openbare literatuur worden toegepast. Uit de beschikbare gegevens worden ecotoxicologische eindpunten geselecteerd voor het afleiden van MTR waarden.

Er worden twee methoden gebruikt voor afleiding van de MTR waarden: de statistische extrapolatie methode ('refined effect assessment') van Aldenberg en Slob (1993) en extrapolatie methode die gebruik maakt van extrapolatiefaktoren ('preliminary effect assessment') volgens de 'Technical Guidance Documents' (ECB, 1996). De keuze welke methode wordt toegepast (statistisch of extrapolatiefaktoren), wordt bepaald door de hoeveelheid en de aard van de beschikbare ecotoxicologische gegevens. Voor de statistische extrapolatie zijn minimaal vier lange termijn chronische toxiciteitsgegevens nodig voor vier verschillende soorten. Indien minder gegevens beschikbaar zijn wordt gebruik gemaakt van extrapolatiefaktoren. De grootte van de extrapolatiefaktor neemt toe naarmate de hoeveelheid beschikbare gegevens afneemt.

MTR waarden voor bodem en sediment kunnen ook afgeleid worden op indirecte wijze. Hierbij wordt dan gebruik gemaakt van de evenwichtspartitie methode (Ep methode). Deze methode schat de concentratie in de bodem en het sediment aan de hand van partitiecoëfficiënten. De voornaamste aanname in het toepassen van deze methode is dat er evenwicht is tussen de hoeveelheid stof geabsorbeerd aan het organisch materiaal en de hoeveelheid stof (niet voor metalen) opgelost in de water fase. De Ep methode wordt ook gebruikt voor intercompartimentale afstemming. Dit is nodig omdat transport van de stof tussen de verschillende milieucompartimenten optreedt. Voor stoffen met een log $K_{ow} > 5.0$, slechte uitscheiding of sterk accumulerende eigenschappen wordt er gekeken of er een potentieel risico voor doorvergiftiging is, en in voorkomende gevallen wordt daarmee rekening gehouden.

SUMMARY

It is possible at the moment in the Netherlands that in the framework of the admission of plant protection products and biocides different Maximum Permissible Concentrations (MPCs) are operative than those derived in the framework of "Derivation of Integrated Environmental Quality Standards". It is undesirable that two or three different MPCs for the same compound coexist. Therefore, the procedures for derivation of MPCs for admission policy of plant protection products and biocides and the setting of environmental quality standards are harmonised. MPCs for plant protection products and biocides are derived the moment a product is (re)registered, even when the "unless" criteria of the "Decree on Environmental Requirements on Pesticides Registration" do not apply (VROM, 1997).

A search profile for literature is presented. In the process of derivation of harmonised MPCs, the criteria of Mensink *et al.* (1995) and Kalf (1996) will be used for evaluating the confidential studies from the admission dossier and public literature. From the available data a selection is made. Which data are used for MPC derivation depends on the amount, reliability and the kind of data.

Two methods will be used to derive harmonised MPCs from ecotoxicological studies (direct method): the refined effect assessment method (Statistical extrapolation according to Aldenberg and Slob, 1993) and the preliminary effect assessment method using assessment factors of the Technical Guidance Documents (ECB, 1996) and the modified EPA method (OECD, 1992). Since long term chronic toxicity data are preferred the aim is to apply the refined effect assessment method. This method can only be applied if at least four long term NOEC values for four species are available. If these data are not available the preliminary effect assessment method is applied. The assessment factors express the uncertainties in data availability (higher factors for less data).

MPCs for soil and sediment can also be derived indirectly from the MPC water if experimental data are lacking. The applied method is the equilibrium partitioning method (Ep-method). This method estimates the concentration in the soil or sediment using partition coefficients and is based on the assumption that an equilibrium exists between the chemical sorbed to the solid phase and the pore water. The Ep-method is also used to harmonise the MPCs of the individual environmental compartments, because transport of compounds between environmental compartments is assumed. Secondary poisoning is taken into account if Log K_{ow}>5 or low degradation or high accumulation rates are expected. In this case the MPCs based on the direct methods will be adjusted due to accumulation potential of a compound in top predators.

1 INTRODUCTION

1.1 History

In the framework of the admission of plant protection products and biocides different Maximum Permissible Concentrations (MPCs) are operative than those derived in the framework of the project "Setting of Integrated Environmental Quality Standards (abbreviation in Dutch: INS)". It was concluded that it is undesirable that different MPCs for the same compound coexist(VROM, 1998 (VenW, 1997). Therefore, the procedures for setting of MPCs for admission policy of plant protection products and biocides, and the setting of environmental quality standards have to be harmonised. The ministry of VROM[1] developed a framework in which the responsibilities concerning the derivation of harmonised MPCs are laid down. In this harmonised procedure MPCs are derived for soil, water and sediment. MPCs for plant protection products and biocides are derived the moment a product is (re)registered, even when the "unless" criteria of the "Decree on Environmental Requirements on Pesticide Registration (in Dutch: Besluit Milieutoelatingseisen Bestrijdingsmiddelen (BmB)) do not apply (VROM, 1997).

1.2 Parties and their responsibilities

The primary responsibility for setting MPCs for plant protection products and biocides is laid down at the Dutch Board for the Authorisation of Pesticides (in Dutch: het College voor de Toelating van Bestrijdingsmiddelen (CTB)). The harmonised procedure and the methodology will be legally embedded in the BmB. The procedure for derivation of scientific MPCs had to be agreed upon by an interdepartmental Steering Group (in Dutch: Stuurgroep INS) and the CTB, and was accepted by the Steering Group Pesticide Policy (in Dutch: Stuurgroep Bestrijdingsmiddelenbeleid (SGB)). The methodology for derivation of MPCs was originally developed at the Centre for Substances and Risk assessment (CSR) of the National Institute of Public Health and the Environment (RIVM). The technical aspects are therefore largely based on the sources and expertise within RIVM/CSR. The CTB will be responsible for subcontracting third parties, such as the RIVM, that perform the derivation of the MPCs according to the procedures laid down in this harmonised protocol. MPC always need to be verified by the Advisory Group 'Setting of Environmental Quality Standards' (Abbreviation in Dutch OZBG voor ecologische risico's).

[1] Letter of Ir. M. Bovenkerk (VROM/DGM/SVS) to SGB, IWINS and CTB, dd. November 4, 1997, SVS/SN/0536.

1.3 MPC protocol

Prior to the development of this report the differences in the methodology used for MPC derivation between the registration policy of plant protection products and biocides and the setting of environmental quality standards were evaluated. The decisions derived from this work are embedded in the harmonised protocol. The notice with discussion points can be found in Annex 2.

In this report the procedure for the setting of harmonised MPCs is laid down. No extensive description on search methodology, technical aspects and/or background information on MPC derivation is given in this document. Where possible it is referred to Mensink *et al.* (1995) and Kalf (1996). If a specific item has changed due to the harmonisation process or the mentioned documents do not give sufficient guidance, the item is further explained in the present document. It should be stressed here that to be able to derive MPCs Mensink *et al.* (1995) and Kalf (1996) are essential references. In Figure 1 a flowchart of the procedure of MPC setting is presented. Figure 2 focuses on the dotted section from Figure 1.

The procedure in Figure 2 contains the following elements:

1. A direct method for derivation of MPCs. The direct method uses ecotoxicological endpoints to calculate MPCs for water, soil and sediment.
2 An indirect method for derivation of MPCs. The indirect method calculates the MPCs for soil and/or sediment using the equilibrium partitioning method or the secondary poisoning approach.

If MPCs for soil and sediment are derived using the direct method the MPCs should be harmonised with the MPCs derived from the indirect methods. The lowest or the most reliable MPC is chosen as the 'final' MPC value. If no MPC for the aquatic compartment is available the Ep-method will be be used to calculate the MPC water from the MPCs for soil or sediment.

The structure of this report is based on the chronological steps needed for derivation of harmonised MPCs. Chapter 2 deals with the literature search methodology. The search profiles for obtaining public literature can be found in Annex 1. Chapter 3 deals with the evaluation of ecotoxicological studies. Also included in this chapter is a section on reliability indicators and usefulness criteria that will be allocated to the individual studies. Chapter 4 deals with the criteria for selection of ecotoxicological endpoints for MPCs derivation. Finally, chapter 5 deals with the methods used for derivation of harmonised MPCs: the refined effect assessment method, the preliminary effect assessment method (Technical Guidance Document and modified EPA method), the equilibrium partitioning

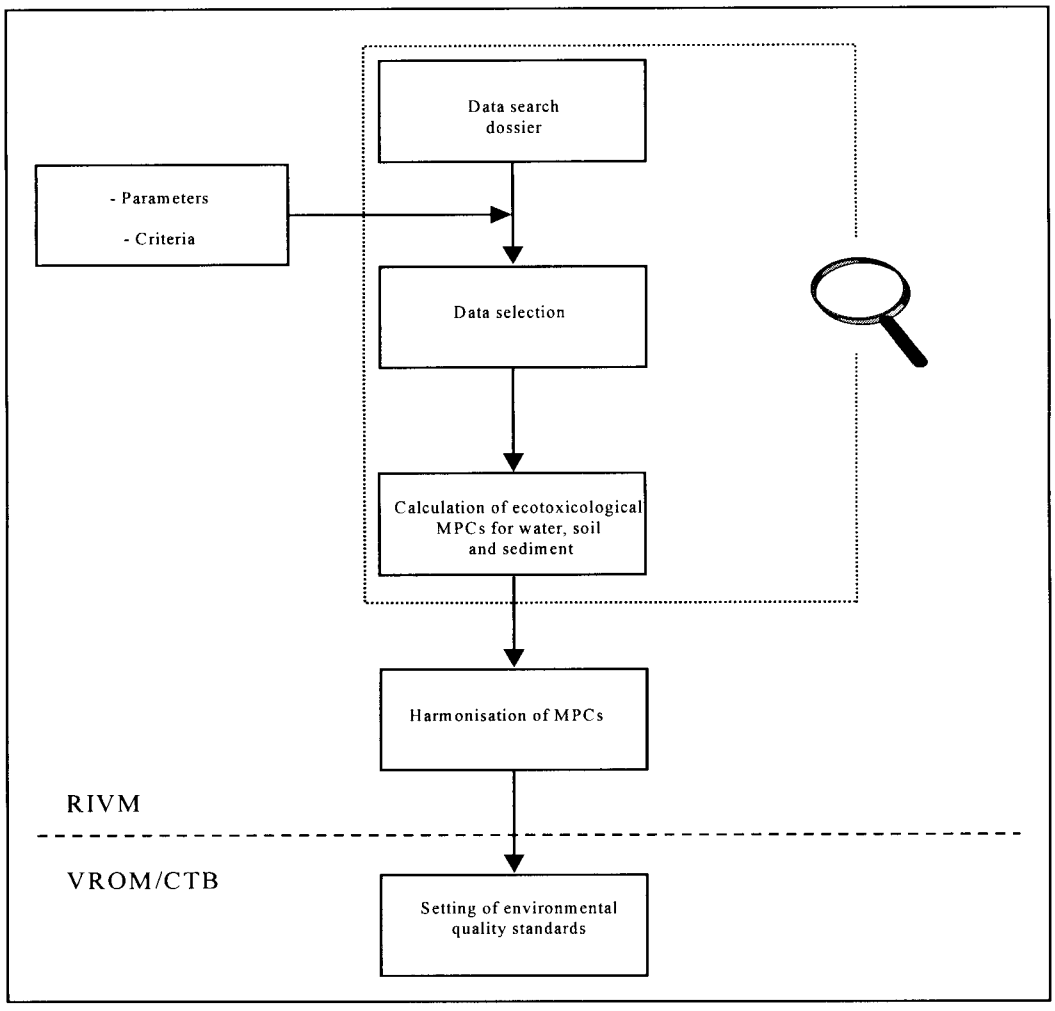

Figure 1: Schematic presentation of the process of deriving environmental quality standards.

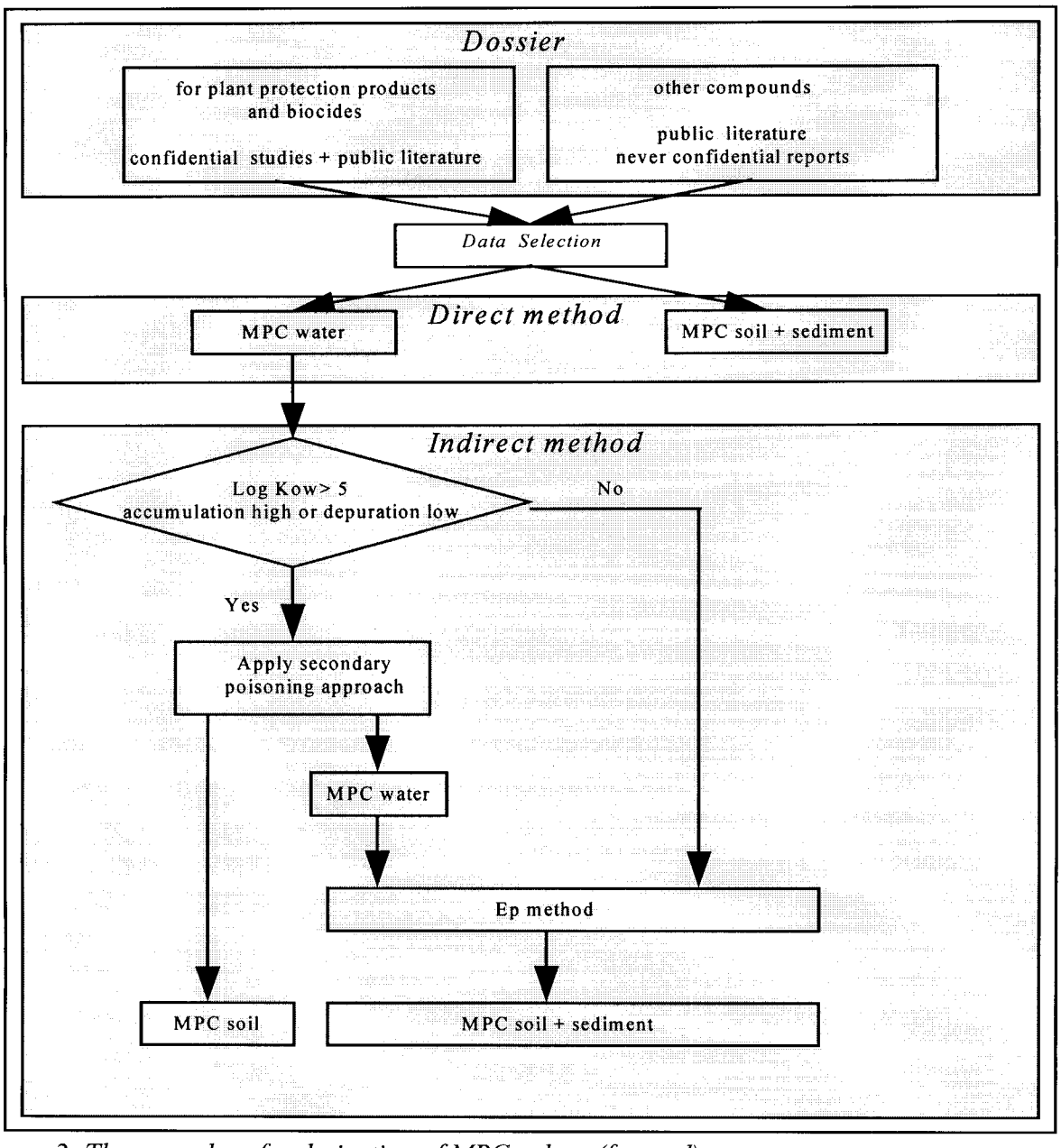

Figure 2: The procedure for derivation of MPC values (focused).

method and the methods to incorporate secondary poisoning in MPC derivation. In Annex 2 the notice from the Ministry of VROM with discussion points can be found. The abbreviations used in this report can be found in the glossary in Annex 3. In Annex 4 the consequences of using the assessment factors from the TGD (ECB, 1996) are discussed. In Annex 5 the reference lines for calculating background concentration for metals are given. Finally, in Annex 6 an alternative method for incorporating secondary poisoning is presented, that might be of importance in the future.

2 LITERATURE SEARCH METHODOLOGY

In this chapter the methodology for collection of literature according to the harmonised procedure is outlined. Some adjustments to the method outlined in Kalf (1996) are made. These adjustments are discussed with the Dutch Board for the Authorisation of Pesticides (CTB).

For plant protection products and biocides an admission dossier (containing confidential studies compulsory for admission and additional public literature) is received from the CTB. For MPC derivation for compounds other than 'plant protection products and biocides' the data set is formed entirely by public literature. MPC values will be derived weighing all relevant data. In §2.1 the literature sources that need to be consulted are enumerated. The literature search profiles underlying the on-line search actions can be found in Annex 1 of this report. Finally, in §2.2 the actual search process and targets are outlined.

2.1 Literature sources

The admission dossier for pesticides and biocides (containing the confidential studies compulsory for admission and the additional public literature) is received from the CTB. Which confidential studies are enclosed in the admission dossier can be found in the application form A of the CTB (CTB, 1995). Existing monographs prepared by CTB or EU are considered of equal value.

The public literature sources for single-species toxicity data and data on soil/water and sediment/water partition coefficients are:

- On-line search in the bibliographic databases Biosis (ecotoxicological data and partition coefficients), TOXLINE (for mammalian data) and Chemical Abstracts (data on partition coefficients). The lay out of the search profiles is developed to use the host 'Deutsches Institut für Medizinische Dokumentation und Information (DIMDI), except for Chemical Abstract for which the host DIALOG is used (see Annex 1).
- Libraries such as: the library of the Centre for Substances and Risk Assessment, the National Institute of Public Health and the Environment and the CTB library. Grey literature can be searched for depending on time and budget. In Kalf (1996) internal CSR literature sources are mentioned. These sources can only be consulted by CSR employees, but the information which is stored in the CSR literature can also be obtained from public sources.
- All secondary literature found will be used to find primary literature (the so-called retrospective literature search method). The aim is to be as complete as possible. In principle only primary literature is used for MPC derivation!

2.2 Search process and targets

The search process is based on the INS methodology (Kalf, 1996). In INS the on-line search is based on the year of publication of the most recent 'reliable' review. Since reliability is not easy to determine in this case, reliability should be read as 'complete'. Whether or not a review represents the state of the art is judged on a case-by-case basis and relies on expert judgement. If no review is available INS advises to start the search from 1970 or from the beginning of the database in question. However, based on expert judgement also other starting points can be used.

In the harmonised procedure MPCs are derived, using the direct method, for water, soil and sediment based on ecotoxicological data for all species[2] living in these environmental compartments. Ecotoxicological data for birds and mammals and BCF values for fish, mussels and worms are only searched for when secondary poisoning needs to be assessed (Search actions are only initiated if: the $\log K_{ow}$ of a compound/substance is higher than 5.0 or if the compounds has a very low metabolisation and/or excretion rate or, if in case of (organo) metals: if the consulted literature confirms the expectation for secondary poisoning; see also §5.4 of this report). Partition coefficients are needed for applying the equilibrium partitioning method (see § 5.3 of this report).

Because in Kalf (1996) the text is divided into sections a summary is given below for what data is searched for:

- Ecotoxicological studies for all aquatic species, marine and freshwater;
- Ecotoxicological studies for all soil organisms, enzymatic activities and microbial processes;
- Ecotoxicological studies for all sediment dwelling organisms;
- Ecotoxicological studies for all birds and mammals;
- Partition coefficients (for applying the equilibrium partitioning method).

[2] 'All species' refer to: all species including so-called target or pest species. For further discussions on this subject it is reffered to Annex 2 (Harmonising the protocol for MPCs; bottlenecks and discussion points) of this document.

3 EVALUATION OF ECOTOXICOLOGICAL STUDIES

When evaluating ecotoxicological studies for effect assessment there are criteria that should be kept in mind, that may have direct impact on the derived MPC. For the evaluation of the ecotoxicological studies Mensink *et al.* (1995) developed summary tables. These summary tables represent the way studies are summarised in the process of admission of plant protection products. In Kalf (1996) also evaluation criteria are developed. In principle there are not many differences in the criteria between the two frameworks. Therefore, only the differences in criteria between the two frameworks are worked out in this document. Because the criteria are reported more extensively in Mensink *et al.* (1995) than in Kalf (1996), the former should be used.

A reliability index (RI) is allocated to studies as a measure for the coherence with the developed criteria (for Reliability and usefulness of studies see § 3.1). Instructions on compound specific background information can be found in §3.2. Section 3.3 deals with the procedures for derivation of the toxicity endpoints (short term L(E)C50s and long term NOECs) from the ecotoxicological studies.

3.1 Reliability and usefulness of studies

Confidential reports and public literature have different status for the regulatory authorities on pesticide registration as public literature generally does not comply with the data requirements for pesticide registration. However, this is not a problem for MPC derivation purposes. The studies, confidential reports and public literature, will be summarised according to the criteria found in Mensink *et al.* (1995). If the studies are judged useful and reliable they will be used to derive MPCs (see Figure 3). For reliability indicators see §3.1.1.

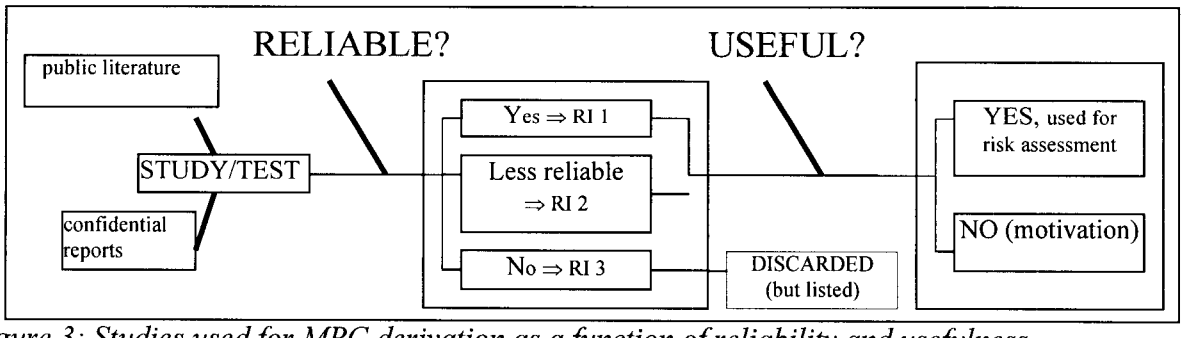

Figure 3: Studies used for MPC derivation as a function of reliability and usefulness

Reliability Indicators (RIs) are used for the designation of the reliability of a study. The overall RIVM/CSR concept for RIs, respecting confidential reports is laid down in Mensink *et al.* (1995). In Table 1 the RI concept is laid down for both confidential reports and public literature. This concept refers to the reliability of any test or study, irrespective where it is used for. Final

purposes of such qualifications are *e.g.* to select a particular set of publications with relevant endpoints that are useful for environmental risk assessment, for (re)registration purposes, or for MPC derivation.

Table 1: Reliability indicators for qualifying studies

Reliability indicators	Definition	Description
		Public literature/Confidential reports
1	RELIABLE	the methodology and the description are in accordance with internationally accepted test guidelines and/or the instructions in Mensink *et al.* (1995)
2	LESS RELIABLE	the methodology and/or the description are less in accordance with internationally accepted test guidelines and/or the instructions in Mensink *et al.* (1995)
3	NOT RELIABLE	the methodology and/or description are not in accordance with internationally accepted test guidelines and/or the instructions in Mensink *et al.* (1995)

3.2 Compound specific background information

For derivation of MPCs it is essential to obtain background information such as physical/chemical properties and properties concerning degradation/metabolite formation. The reason that this background information is essential is that the environmental fate and behaviour of compounds might influence the outcome of standard laboratory test and thus influences the MPCs. For the compound specific background information that is necessary to derive MPCs one is referred to Kalf (1996).

Some examples on the importance of compound specific background information:

- Assuming a volatile compound; a *Daphnia* test is performed in a static open system in which the test concentrations were not measured and the NOEC is reported as a nominal exposure concentration. It is in this case impossible to estimate the actual exposure concentration, since an unknown fraction of the volatile substance will have been evaporated from the test system, which will cause an unknown decrease in the actual concentration.
- Assuming a rapidly degrading compound in the same test system as the previous example. In this case the observed toxicity might be caused by the metabolites instead of the parent compound.

Physical/chemical properties

The following physical/chemical properties are of importance as background information for MPC derivation. Extensive guidance on how to apply these physical/chemical properties can be found in Kalf (1996).

- Water solubility
- Henry's law constant
- Octanol/water partition coefficients (Log K_{ow}).
- Solid/water partition coefficients ($K_{s/l}$)

When soil toxicity data are insufficient to derive an MPC, it can be derived from aquatic toxicity data by means of the equilibrium partitioning method (Slooff, 1992). To apply this method the solid/water partitioning coefficient ($K_{s/l}$) is needed. The reader is referred to the INS document (Kalf, 1996) for further instructions.

When deriving MPCs all information concerning $K_{s/l}$ and 1/n is useful. Concentration dependent sorption behaviour is however not taken into account in standard models of leaching to groundwater. For these calculations (that are not within the scope of INS, but within the scope of pesticide registration) $K_{s/l}$ are only selected if the Freundlich exponent (1/n) is within the range of 0.7 - 1.1 (Mensink *et al.*, 1995).

Properties concerning degradation/metabolite formation

Guidance on degradation processes such as: hydrolysis, photolysis and biodegradation and metabolite formation can be found in Mensink *et al.* (1995) and Kalf (1996).

Once it is established that hydrolysis is the (main) cause for the high loss, the second question is if the metabolite(s) should have been tested instead of the parent compound, or it can be concluded that testing of both parent compound and metabolite(s) is necessary. In Kalf (1996) the criteria of Whitehouse and Mallet (1993) are used. In Mensink *et al.* (1995) these criteria were slightly changed. It is decided for derivation of harmonised MPCs to use the criteria proposed in Mensink *et al.* (1995), see Table 2.

Table 2: Dissipation criteria for the selection of the test substance in aquatic toxicity testing.

DT_{50}	Selection
24 h	the test is started with the parent substance
<4 h	test(s) is (are) started with metabolites
4-24 h	expert judgement

3.3 Derivation of ecotoxicological endpoints

The methodology used for derivation of endpoints from ecotoxicological studies is described in Kalf (1996). In water the dissolved fraction is always equal to 1.

Recalculating terrestrial toxicity endpoints to standard soils

The data for terrestrial species and for microbial processes/enzymatic activity of organic chemicals and metals are normalised to standard soil. In Kalf (1996) a percentage organic matter of 10 is used, whereas 5% organic matter is the standard soil for plant protection products. It is decided that MPCs will be presented for both standard soils.

Organic compounds

The following equation is used for normalisation to standard soil if organic compounds are tested:

Equation 1: Recalculation of terrestrial toxicity endpoints to standard soil for organic compounds

$$NOEC; L(E)C50_{(ssoil)} = NOEC; L(E)C50_{(\exp)} \frac{o.m._{(ssoil)}}{o.m._{(\exp)}}$$

Legends:
NOEC;$LC50_{(ssoil)}$ = normalised NOEC or LC50 for standard soil,
NOEC;$LC50_{(exp)}$ = NOEC or LC50 for soil as used in the experiment,
$o.m._{(ssoil)}$ = organic matter content of standard soil (5% or 10%),
$o.m._{(exp)}$ = organic matter content of soil used in experiment (%).

If o.m.< 2% the percentage is set to 2%, if o.m.>30 % the percentage is set to 30%.

Metals

For metals the conversion to standard soil is carried out using equation 2. In order to apply this equation, metal specific reference lines are necessary. These reference lines can be found in Crommentuijn *et al.* (1997b, Table 5.1 page 62), see also Annex 5 of this report.

Equation 2: Recalculation of terrestrial toxicity endpoints to standard soil for metals

$$NOEC_{st.soil} = NOEC_{exp.} \times (\text{reference line}^{\#1} / (a+b*\%o.m.) + (c*\%clay)$$

Legends:
$NOEC_{st.\ soil}$ = NOEC standard soil
$NOEC_{exp.}$ = Experimental NOEC
a,b,c = Correction factors for metals
$^{\#1}$ = Reference lines (Crommentuijn *et al.* (1997b), see also Annex 5 of this report)

It should be stressed here that MPCs for metals are calculated as the maximum permissible addition (MPA) plus the natural background concentration (C*b*). The MPA is considered to be the amount of metal originating from antropogenic sources. This means that for individual

ecotoxicological studies in which metals are tested, the NOEC or L(E)C50 should be based on the additional metal concentrations. For a full version of the so called added risk approach it is reffered to Crommentuijn *et al.* (1997b). The MPA for metals and other natural occuring substances is derived analogously as the MPC for organic substances that have no natural background.

4 SELECTION OF ENDPOINTS FOR MPC DERIVATION

Before applying the extrapolation methods for MPC derivation (see chapter 5), a selection has to be made from the available toxicity endpoints. A number of selection criteria are available: Reliability indicators (§4.1) and other criteria for selection of ecotoxicological endpoints, see § 4.2.

4.1 Reliability indicators

No distinction will be made between the confidential studies from the admission dossier and the public literature for MPC derivation. After tagging RIs to the individual tests, only those tagged with RI 1 or RI 2 are selected for the actual MPC derivation and those tagged with RI 3 are not used. It is of particular importance to make a clear dividing line between RI 1 and 2 on one, and RI 3 on the other hand.

4.2 Selection of ecotoxicological endpoints

As mentioned in §2.3 ecotoxicological endpoints of all species (see Annex 2) will be used for MPC derivation.

For the procedure of deriving MPCs for the aquatic environment the following point of view is used: differences may be present between freshwater and marine species. If possible, a comparison of the sensitivity between freshwater and marine species should be made. If no differences are found, it is considered justified to derive one MPC which is based on the combined ecotoxicological data set for freshwater and marine species. If significant differences can be demonstrated between marine and freshwater species both MPCs will be derived.

In the extrapolation methods presented in chapter 5 only one toxicity endpoint per species is used as input for the extrapolation methods. If more than one endpoint for a species or process is available, a selection has to be made which value to use in the extrapolation. The criteria summarised below are derived from Kalf (1996):

- Only toxicological criteria which may affect the species at the population level are taken into account for derivation of the MPC. In general these are survival, growth and reproduction.
- If for one species several results for the same toxicological endpoint are available, the endpoints are averaged by calculating the geometric mean.
- If for one species several results with different pH, DOC, T (°C) or hardness are available, the endpoints are selected based on knowledge on the natural habitat of the tested species and based on specific fate and behaviour of the compound in question.
- If for one species several results, fore different toxicological endpoints are available, the lowest value is selected.

- In some cases toxicity endpoints are available for effects on different life stages. If it becomes evident that a certain lifestage is more sensitive, the most sensitive endpoint is used in the extrapolation.
- For the data on microbial processes and enzymatic activities, more than one value per process can be included in the extrapolation method. The reason is that an experiment which is performed using different soils will have a different population of bacteria and other micro-organisms.

5 DERIVATION OF MPC VALUES

In Chapter 1.3 an introduction on the derivation of MPCs is given.
For derivation of MPCs directly from ecotoxicological endpoints two different methods are used: the refined effect assessment method (§5.1) and the preliminary effect assessment method (§5.2). Because long term chronic data are preferred above short term acute data the aim is to apply the refined effect assessment method. However the application of this method is based on data availability: at least four NOEC values are needed for four different taxonomic groups of organisms. If these data are not available the preliminary effect assessment method is applied. In this case in principle the TGD is applied. In Figure 4 the direct method for MPC derivation is presented in a decision scheme.

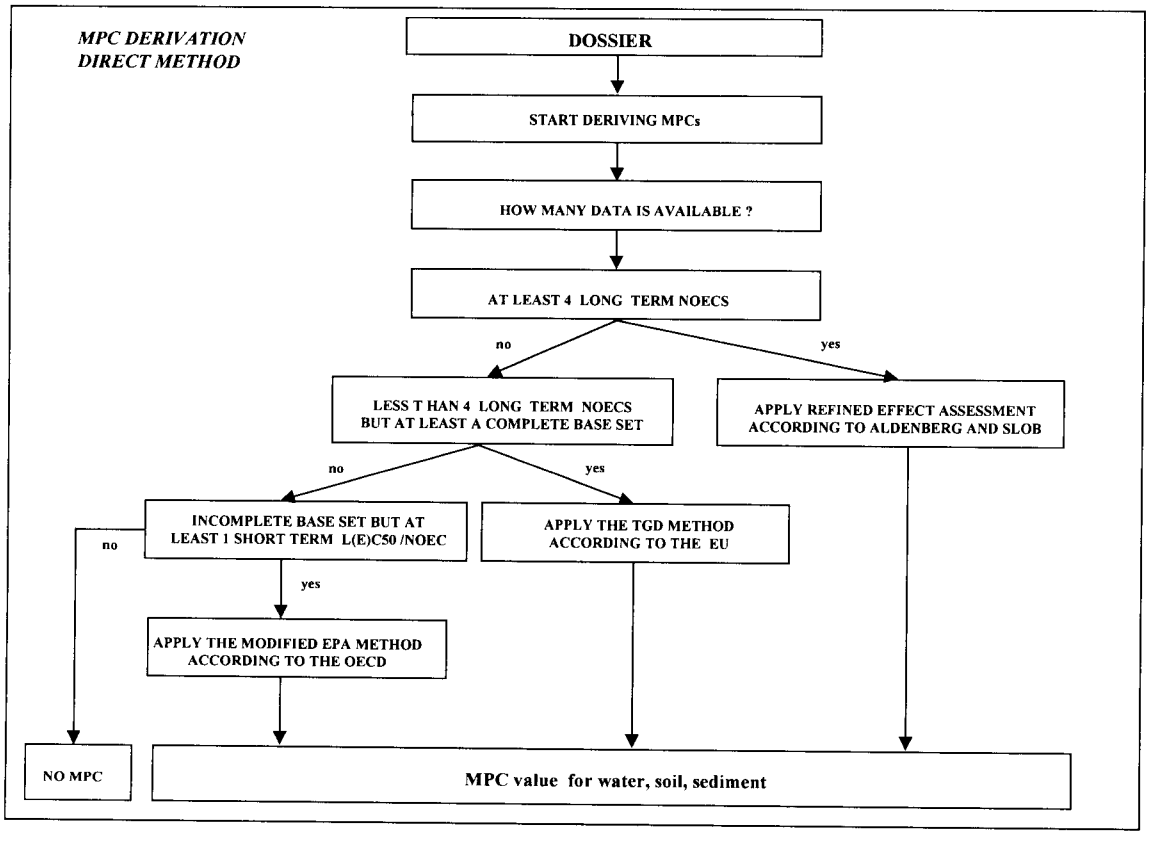

Figure 4: The direct method for MPC derivation.

MPCs for sediment are derived indirectly from the MPCwater even if experimental data are available. This is done using the equilibrium partitioning method (Ep-method; see §5.3). The MPCsoil is derived indirectly from the MPCwater if experimental data are lacking for soil. Inversely, if no toxicity data for the aquatic compartment are available the Ep-method will be be used to calculate the MPCwater from the MPCsoil. For pesticides however, experimental data for soil and water will always be available due to the dossier requirements.

In §5.4 the methodology is given to assess the risk for secondary poisoning. When this applies (logKow >5) the data set for water and soil may be modified (extended) based on the accumulation potential of a compound in top predators. This step is actually performed at the selection of ecotoxicological endpoints and leads to "modified" MPCs.

The Ep-method is also used to harmonise the MPCsoil with the MPCwater (not the other way around). The reason to harmonise these MPCs is the occurrence of transport of compounds from one environmental compartment to another. The lowest or the most reliable MPC is chosen as the 'final' MPC value.

The MPCs for metals and other naturally occuring substances are calculated as the maximum permissible addition (MPA) plus the natural background concentration (C*b*). The MPA is considered to be the amount of substance originating from antropogenic sources. This approach is called the added risk approach. For a full version of the approach it is reffered to Crommentuijn *et al.* (1997b).

5.1 Refined effect assessment: statistical extrapolation

The aim of environmental quality standards is that the MPC is set at a level that protects all species in an ecosystem. However, in order to be able to use extrapolation methods like the one of Aldenberg and Slob, a 95% protection level is chosen as a sort of cut-off value (VROM, 1989). When deriving the MPC, the risk of a substance for the ecosystem can be defined as the potentially affected fraction of all species in this ecosystem (PAF). The concentration corresponding to a PAF of 0.05 is defined as the MPC, and can be derived using statistical extrapolation methods.

The method of Aldenberg and Slob (1993) is used if long term NOECs for four or more different taxonomic groups are available. This method assumes that the NOECs used for estimating the distribution, fit the log-logistic distribution. The advantage of the log-logistic distribution is that it allows the analytical evaluation of the cumulative distribution of PAF by integration. See Equation 3.

Equation 3: Calculation of the PAF for all possible species at concentration x

$$PAF(x) = 1/(1+ exp ((\alpha-x)/\beta))$$

Legend:
PAF(x) = potentially affected fraction of all possible species at conc. x
α= mean value of the log-logistic distribution
β = scale parameter of the log-logistic distribution
x = log(c): logarithm of the concentration

The log-logistic distribution can be characterised by α and β. The α indicates the mean value of the distribution which determines the location of the distribution on the concentration axis (log(NOEC) or log(c)) and β is the scale parameter of the distribution which determines the width or shape of the distribution and is equal to approximately half times s ($\beta = s \sqrt{3}/\pi$).

PAF(x) has a value between 0 and 1 and is the fraction of species that have log(NOEC) values smaller than x. The MPC is set at a level that protects 95% of all possible species in an ecosystem (VROM, 1989). This implies that PAF is equal to 0.05. The corresponding concentration can be calculated with a 50% and 95% confidence level. In the Netherlands the MPC is set equal to the former value. This concentration (or another concentration, corresponding to another fraction of species unprotected) can be derived by rewriting equation 3 into equation 4:

Equation 4: Rearrangement of equation 3 for a concentration x

$$x = \alpha- \beta \ln ((1-PAF)/PAF)$$

Legend:
PAF(x) = potentially affected fraction of all possible species at conc. x
α = mean value of the log-logistic distribution
β = scale parameter of the log-logistic distribution
x = log(c): logarithm of the concentration

Calculations can be made using a spreadsheet and the appropriate statistical tools. In USES2.0 (RIVM *et al.* 1998), the statistical extrapolation is performed for aquatic organisms when sufficient data are entered. It is recommended to use USES2.0.

5.2 Preliminary effect assessment

If long term NOECs for less than four species from four different taxonomic groups are available, the preliminary effect assessment method is used. It is decided that for the derivation of harmonised MPCs in principle the assessment factors of the ECB (1996), laid down in the Technical Guidance Documents (TGD), will be used[3]. How to apply assessment factors to the

[3] Up to and until 1998 INS used the modified EPA method (OECD, 1992).

available toxicity data is clearly depicted in the European Union System for the Evaluation of Substances manual (EUSES; EC, 1996). The application of the TGD assessment factors, according to EUSES, is presented in Table 3 (aquatic compartment) and Table 4 (terrestrial compartment). The text of the TGD is available in Annex 7.

Aquatic compartment

NOEC refers to long term toxicity tests, L(E)C50 to short term toxicity tests and 'base set' to three L(E)C50 values from acute aquatic toxicity tests, carried out with three organisms each representing a different trophic level. The trophic levels are represented by: algae, *Daphnia* and fish.

Table 3 Assessment factors for aquatic toxicity data following EU/TGD (ECB, 1996); according to EUSES (EC, 1996)

Available data	**Additional criteria**	**TOXaqua**	**AFaqua**
3 L(E)C50s		$LC50aqua_{min}$	1000
3 L(E)C50s (independent of avail. NOECs)	If intermittent release is identified for a stage of the life cycle*	$LC50aqua_{min}$	100
	NOEC from same taxonomic group as $LC50aqua_{min}$?		
1 NOEC additional (not algae!)	yes	$NOECaqua_{min}$	100
	no $LC50aqua_{min}/1000 < NOECaqua_{min}/100$		1000
	no $LC50aqua_{min}/1000 < NOECaqua_{min}/100$		100
	More than one NOEC available?		
2 NOECs additional	yes	$NOECaqua_{min}$	50
	no	$NOECaqua_{min}$	100
3 NOECs algae, *Daphnia* and fish		$NOECaqua_{min}$	10
3 NOECs not algae, *Daphnia* and fish		$NOECaqua_{min}$	10
		$NOECaqua_{min}$	50

* not relevant for derivation of MPCs

There are three exceptions to the rules:

1. Only when long term NOECs on three trophic levels are available, a comparison with data from the (complete) base set is no longer demanded.

2. In case the base set is incomplete, a factor 10 and/or 1000 will be applied to the NOEC and/or L(E)C50, respectively, to derive the MPC (modified EPA method (OECD, 1992)). It should be stressed here that this exception may only be used if the TGD can not be applied. The tables with the EPA assessment factors can also be found in Kalf (1996).

3. It is inferred that for more hydrophobic compounds, short term toxicity data may not be representative, since the time span of an acute test may be too short to reach a toxic internal level. In those cases, base set completeness is not demanded and an assessment factor of 100 may be applied to a chronic test, which should not be an alga test if this is the only chronic test available.

Terrestrial compartment

In the terrestrial compartment a distinction is made between species and (microbial) processes. For both species and processes an MPC is derived. Secondary poisoning applies only for species. The lowest or the most reliable MPC is chosen as the 'final' MPC value for soil, that is compared with the harmonised MPC starting from the MPCwater.

Note that there is no minimum requirement for toxicity data in the TGD as opposed to the base set for the aquatic compartment (table 4).

For pesticides, additional tests will be required if the persistency trigger of DT50soil 90 days is exceeded. For example, additional testing on plants, soil arthropods and fungi may be requested by the CTB.

Sediment compartment

For the sediment compartment the MPC is derived only with the indirect method starting from the MPCwater. Experimental data are only used to verify whether the MPC is protective enough. At present, there is no consent on how to treat the endpoints from the different sediment toxicity tests and there is no concept for a base set (testing of different trophic levels). Consequently, guidance on applying assessment factors still has to be developed.

Table 4 Assessment factors for terrestrial toxicity data following EU/TGD (ECB, 1996) according to EUSES (EC, 1996)

Available data	**Additional criteria**	**TOXterr**	**AFterr**
None		$PNEC_{soil, EP}$	1
	Additional criteria		
1 LC50	$PNEC_{soil, EP} < LC50terr_{min}/1000$	$PNEC_{soil, EP}$	1
	$PNEC_{soil, EP} \geq LC50terr_{min}/1000$	$LC50terr_{min}$	1000
>1 LC50		$LC50terr_{min}$	1000
1 NOEC	$PNEC_{soil, EP} < NOECterr_{min}/100$	$PNEC_{soil, EP}$	1
no LC50s	$PNEC_{soil, EP} \geq NOECterr_{min}/100$	$NOECterr_{min}$	100
1 NOEC	$LC50terr_{min}/1000 < NOECterr_{min}/100$	$LC50terr_{min}$	1000
≥1 LC50s	$LC50terr_{min}/1000 \geq NOECterr_{min}/100$	$NOECterr_{min}$	100
	Same taxonomic group as $LC50terr_{min}$?		
2 NOECs	yes	$NOECterr_{min}$	50
	no	$NOECterr_{min}$	100
3 NOECs	yes	$NOECterr_{min}$	10
	no	$NOECterr_{min}$	50

5.3 Equilibrium partitioning

For both sediment and soil the equilibrium partitioning method (Ep-method) can be applied to derive MPCs if no experimental data are available (indirect method). It should be noted that for pesticides always experimental data will be available, due to the dossier requirements for registration. Besides this the Ep-method is used to harmonise the independently derived MPCs for water and soil.

If no toxicity data for the aquatic compartment are available the Ep-method will be be used to calculate the MPCwater from the MPC for soil. The Ep-method will however not be used to harmonise an MPCwater starting from an MPCsoil. Again, for pesticides always experimental data for the aquatic compartment will be available, due to the dossier requirements for registration.

For a full description of the Ep-method including the concept, uncertainties and discussions underlying the method, the reader is referred to Crommentuijn *et al.* (1997a).

The MPC for sediment and terrestrial species using equilibrium partitioning is calculated using the following Equation:

Equation 5: Calculation of the MPC soil/sediment using the Ep-method

$$MPCcomp_{Ep} = MPCwater * K_{s//(comp)}$$

Legends: $MPCcomp_{Ep}$ = Maximum Permissible Concentration for terrestrial or sediment compartment using the equilibrium partition theory (dry soil or dry sediment)
MPCwater = Maximum Permissible Concentration for water compartment
$K_{s/l(comp)}$ = partition coefficient for standard soil or standard sediment in [l/kg]

5.4 MPCs for compounds with a potential for secondary poisoning

Secondary poisoning is concerned with toxic effects in the higher members of the food chain which result from ingestion of organisms at the different trophic levels that contain accumulated substances.

Two aquatic food chains (water → fish → fish-eating predators and water → mussel → mussel-eating predators) and one terrestrial food chain (soil → earthworm → worm-eating predators) are considered (Van de Plassche, 1994).
All toxicity data, for lower organisms (i.e. fresh- and saltwater organisms for the aquatic food chain and soil organisms of the terrestrial food chain) and for top predators (i.e. birds and mammals) are combined: first all individual NOECs/LC50s for birds and mammals are divided by the BCF to obtain NOECs/LC50s in water or soil. These values are used as input data together with the L(E)C50 or NOEC values for aquatic or soil organisms in the direct method.

The following algorithm is used:

Equation 6: Algorithms to calculate the effect concentration (EC) due to secondary poisoning

$$ECwater = EC_{bird;mammal} / BCF_{fish,\ mussel}$$

$$ECsoil = EC_{bird;mammal} / BCF_{worm}$$

The effect concentration (EC) can be a NOEC or an LC50. The EC is based on toxicity data for predators like birds and mammals. Preferably, this should be data for fish-eating birds and mammals. However, these data are seldomly available. Therefore, data on other bird and mammalian species have to be used.

BCF stands for Bioconcentration Factor[4]. For water, two BCF are used: fish and mussel. This will result in two ECwater values. The most critical ECwater per species is selected for further calculations.

Toxicity data for birds and mammals result in LC50 (e.g. 5 days dietary study with birds) or NOEC/NOAEL values (e.g. 28 days oral study with rats). If results are expressed in mg/kg body weight they should be converted to mg/kg food using conversion factors (table 6).

Table 6: Conversion factors for recalculation of body weight concentrations to concentrations in food; birds and mammals (ECB, 1996)

Species	**Conversion factor**
Canis domesticus:	40
Macaca spec.:	20
Microtus spec.:	8.3
Mus musculus:	8.3
Oryctolagus cuniculus:	33.3
Rattus norvegicus > 6 weeks old:	20
Rattus norvegicus < 6 weeks old:	10

The BCF can be measured or calculated. The static BCF is the ratio between the concentration in the organism and the concentration in a steady-state (sometimes also called equilibrium) situation. When uptake (k_1) and depuration (k_2) kinetics are measured, the dynamic BCF can be calculated from the quotient of the uptake and depuration rate constants.

Equation 7: Calculation of the BCF from the quotient of the uptake and depuration rate constants.

$$BCF = C_{organisms} / C_{water} \text{ or } k_1 / k_2$$

A geometric mean is calculated from the BCF values (fish or mussels) available. If more than one value is available on a single species a geometric mean is calculated first, before an overall geometric mean is calculated.

If measured BCF for fish or mussel are not available the BCF can be predicted from the relationship between the K_{ow} and BCF. The following relationships are used for fish and mussels:

[4] Bioconcentration is the net result of uptake, distribution and elimination of a substance in an organisms due to water-borne exposure, whereas bioaccumulation includes all routes, i.e. air, water, soil and food. Biomagnification is the accumulation and transfer of chemicals via the food chain, resulting in an increase of the internal concentration in organisms at the higher levels in the trophic chain.

Equation 8 + 9: Calculation of the BCF from the log K_{OW}

$$BCF_{fish} \text{ (whole body, fresh weight)} = 0.05 * K_{OW}$$

$$BCF_{mussel} \text{ (whole body, fresh weight)} = 0.013 * K_{OW}$$

At the moment the BCFworm is not derived from an algorithm. For organic compounds a BCFworm of 10 kg/kg is used. For metals experimentally determined BCFs for earthworms are used.

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ACKNOWLEDGEMENTS

The authors wish to thank D. Sijm, A. van Wezel, E.J. van de Plassche and T. Crommentuijn of the Centre for Substances and Risk Assessment (CSR) and J. de Rijk and M. van der Weijden of the Ministry of Housing, Spatial Planning and the Environment (abbreviation in Dutch: VROM) for critically reviewing this report.
R. Posthumus of CSR and J. Heuver of the Dutch Board for the Authorisation of Pesticides (abbreviation in Dutch: CTB) are thanked for their contributions to the literature search profiles in Annex 1.

ANNEX 1 LITERATURE SEARCH PROFILES

Below the search profiles used for literature search are presented.

A Literature search profile for soil organisms and macrophytes

f bc=(13000 or 13100 or 15000 or 15100 or 15500 or 15900 or 25100 or 04718 or 06509)"
f bc=(25305 or 25330 or 51000 or 51300 or 65000 or 65400 or 75202 or 75402 or 04716)"
f bc=(25345 or 25795 or 25880 or 25840 or 25890 or 26260 or 26285 or 75403 or 06508)"
f bc=(26330 or 26775 or 26865 or 26915 or 75100 or 75112 or 61000 or 75400 or 06503)"
f bc=(61200 or 75200 or 75204 or 75300 or 75304 or 75306 or 75312 or 75352)"
f bc=(75320 or 75344 or 04710 or 04812 or 06704 or 04500 or 06112 or 04510) or minerali#ation"
f (nitrifying or nitrification or denitrification or nitrogen fix? or ammonification)/(ti;ut)"
f nitrobacter or nitrococcus or nitrosomonas or bc=(05800 to 05830) or bc=(08800 to 08851)"
f (phosphatase or invertase or urease or amylase)/(ti;ut) and soil#/(ti;ut)"
f (dehydrogenase or oxygen consumption or respiration)/(ti;ut) and soil#/(ti;ut)"
f (photosynthesis or atp or adenosine triphosphate)/(ti;ut) and soil#/(ti;ut)"
f atpase/(ti;ut) and soil#/(ti;ut)"
f 1 to 12"
f sc=(07506 or 07518 or 22501 or 22506 or 37015 or 40000 or 52801)"
f 13 and 14"
f terrestr? or ?soil# or sediment# or sand# or peat or clay or laom# or organic matter"
f 15 and 16"
f (reproduct? or inhibit? or impact or hazard? or risk# or suppression)/ti"
f (influence# or response# or susceptibilit? or interaction# or effect or effects)/ti"
f (mortalit? or lethal? or survival or growth or tolerance or sensitivit? or intoxication)/ti"
f ec50 or lc50 or noec or matc or pnec or pec or treshold limit or ld50"
f (toxic? or ecotoxic?)/(ti;ut)"
f 18 to 22"
f 17 and 23"
f 24 not la=(ru or ch or cz or it or po or sp or ja or hu)"
f 25 not (removal or remediation or biodeterioration or deterioration)"
f 26 not (bioremediation or soil cleanup)"

B Literature search profile for aquatic organisms

f bc=(13000 or 13100 or 13300 or 13500 or 13700 or 13900 or 14100)"
f bc=(14300 or 14700 or 35100 or 35200 or 35000 or 39000 or 41000)"
f bc=(45000 or 45300 or 51600 or 51000 or 61000 or 61200 or 61500)"
f bc=(65000 or 65500 or 75100 or 75102 or 75108 or 75110 or 75112)"
f bc=(75114 or 83000 or 83100 or 83300 or 83400 or 83500 or 85200)"
f bc=(85206 or 25340 or 25395 or 75314 or 75342 or 75318 or 75300)"
f bc=(75338 or 85300 or 85304 or 85306 or 61600 or 65200)"
f water boatman or waterboatman or photobacterium or pseudomonas"
f 1 to 8"
f 9 not (drosophila or fruit fly or fruit flies)"
f sc=(07502 or 07510 or 07512 or 07514 or 22501 or 22506 or 37015)"
f sc=(07506 or 07516)"
f 11 or 12"

f 10 and 13"
f water# or freshwater# or fresh water# or pond# or lake# or river# or sea"
f seas or ocean? or estuar? or saltwater# or salt water# or brackish or marine"
f saline or brine or seawater or tidal or coast? or (aquatic or salinity)/ti"
f 15 to 17"
f 14 and 18"
f (reproduct? or inhibit? or impact or hazard? or risk# or suppression)/ti"
f (influence# or response# or susceptibilit? or interaction# or effect or effects)/ti"
f (mortalit? or lethal? or survival or growth or tolerance or sensitivit? or intoxication)/ti"
f ec50 or lc50 or noec or matc or pnec or pec or treshold limit or ld50"
f (toxic? or ecotoxic?)/(ti;ut)"
f 20 to 24"
f 19 and 25"
f 26 not la=(ru or ch or cz or it or po or sp or ja or hu or bu)"

C Literature search profile for birds

f bc=(85500 or 85504 or 85506 or 85514 or 85518 or 85520 or 85522 or 85524 or 85526)"
f bc=(85534 or 85536 or 85548 or 85550 or 85554 or 85556 or 85564)"
f 1 to 2"
f sc=(22501 or 22506 or 37015 or 54600)"
f 3 and 4"
f 5 not la=(ch or ja or po or bu pr hu or ru or it or sp or cz)"

D Literature search profile for mammals

Search using the database TOXLINE:
f (rat or rats or mice or mouse or dog or dogs or cat or cats or pig or pigs)/(ti;ct)"
f (hamster# or guinea pig# or mammal? or monkey#)/(ti;ct)"
f 1 to 2"
f (reproduct? or inhibit? or impact or hazard? or risk# or suppression)/ti"
f (influence# or response# or susceptibilit? or interaction# or effect or effects)/ti"
f (mortalit? or lethal? or survival or growth or tolerance or sensitivit? or intoxication)/ti"
f ec50 or lc50 or noec or matc or pnec or pec or treshold limit or ld50"
f (toxic? or ecotoxic?)/(ti;ct)"
f 4 to 8"
f 3 and 9"
f 10 not la=(polh or bulg or japn or chin or span or czec or ital)"

E Literature search profile for partition coefficients

For biosis via the host DIMDI:
f (sorption or adsorption or partitioning or cosolven? or partition)/ti"
f (langmuir or freundlich or sorptive or batch experiment)/ti"
f (equilibri? or isotherm or koc or kd or kp)/ti"
f 1 to 3"
f (soil or soils or sediment? or soil water system? or organic matter or organic carbon)/ti"
f 4 and 5"

f 6 not la=(it or sp or ch or ja or ru or po or cz or hu)"

For chemical abstracts via the host DIALOG:
s sorption or adsorption or desorption or partitioning or cosolven? or partition"
s complexation or langmuir or freundlich or sorptive or bioavailability"
s complex(w)formation or fractionation or precipitation or coprecipitation"
s remobili!ation or equilibri? or partition or isotherm or interaction? or koc or kd or kp"
s S1 or S2 or S3 or S4
s liquid(w)solid or suspended(w)matter or sediment? or suspended(w)particles"
s sludge or soil? or particulate(w)matter or solid(w)phase or liquid(w)phase"
s suspended(w)solid? or suspended(w)material? or interstitial(w)water"
s porewater or groundwater or dissolved(w)matter or dissolved(w)phase"
s third(w)phase or suspended(w)sediment or colloid? or aquifer"
s S6 or S7 or S8 or S9 or S10
s S5 and S11

ANNEX 2 HARMONISING THE PROTOCOL FOR MPCS; BOTTLENECKS AND DISCUSSION POINTS

INTRODUCTION

As a result of historical developments it is possible at the moment in the Netherlands that in the framework of the admission of plant protection products and biocides different MPCs are operative than those in the framework of the project "Setting of Integrated Environmental Quality Standards (abbreviation in Dutch: INS)". A prominent difference between the frameworks is the use of comprehensive, scientific company reports (admission dossier) for pesticide and biocide registration versus the use of articles from scientific journals (public literature) for INS. Also differences are present in the methodologies used in the different contexts. It is concluded that it is undesirable that two or three different MPCs for the same product coexist (NMP3 (VROM, 1998); NW4 (VenW, 1997); second phase MJP-G (Tweede kamer, 1990-1991). Therefore, a framework is developed in the present study in which the responsibilities and the methodology concerning the derivation of MPCs for plant protection products and biocides are laid down. The framework is presented in figure 1.

Since 1998, the Dutch Board for the Authorisation of Pesticides (in Dutch: het College voor de Toelating van Bestrijdingsmiddelen (CTB)) is responsible for determining MPCs for plant protection products and biocides. In 1997 the involved parties agreed on deriving the MPCs for soil and water and if necessary for sediment, the moment a product is (re)registered, even when the "unless" criteria of the "Decree on Environmental Requirements on Pesticide Registration (in Dutch: Besluit Milieutoelatingseisen Bestrijdingsmiddelen (BmB)) do not apply (VROM, 1997)[5].

The harmonised procedure and the methodology will be legally embedded in the BmB. The procedure for derivation of scientific MPCs has to be agreed upon by an interdepartemental Working Group (in Dutch: Stuurgroep INS) and the CTB, and will have to be accepted by the Steering Group Pesticide Policy (in Dutch: Stuurgroep Bestrijdingsmiddelenbeleid (SGB)). The CTB will be responsible for subcontracting third parties that perform the derivation of the MPCs according to the methodology laid down in the harmonised protocol. Because the methodology for derivation of MPCs is developed at RIVM/CSR it is assumed in this document that the technical aspects of the derivation of MPCs are based on the sources and expertise within CSR.

In order to accommodate the aim of consistent MPCs the procedures of INS and the admission assessment need to be harmonised. The Standard Operation Procedures of INS (CSR, 1996) and of the admission assessment (Mensink *et al.*, 1995; CTB, 1993) are compared on the crucial points to find the differences and the bottlenecks. In table 1 the bottlenecks are presented, after which these items are discussed. Where possible a RIVM-CSR/CTB proposal is given.

[5] Letter of Ir. M. Bovenkerk (VROM/DGM/SVS) to SGB, IWINS and CTB, dd. November 4, 1997, SVS/SN/0536.

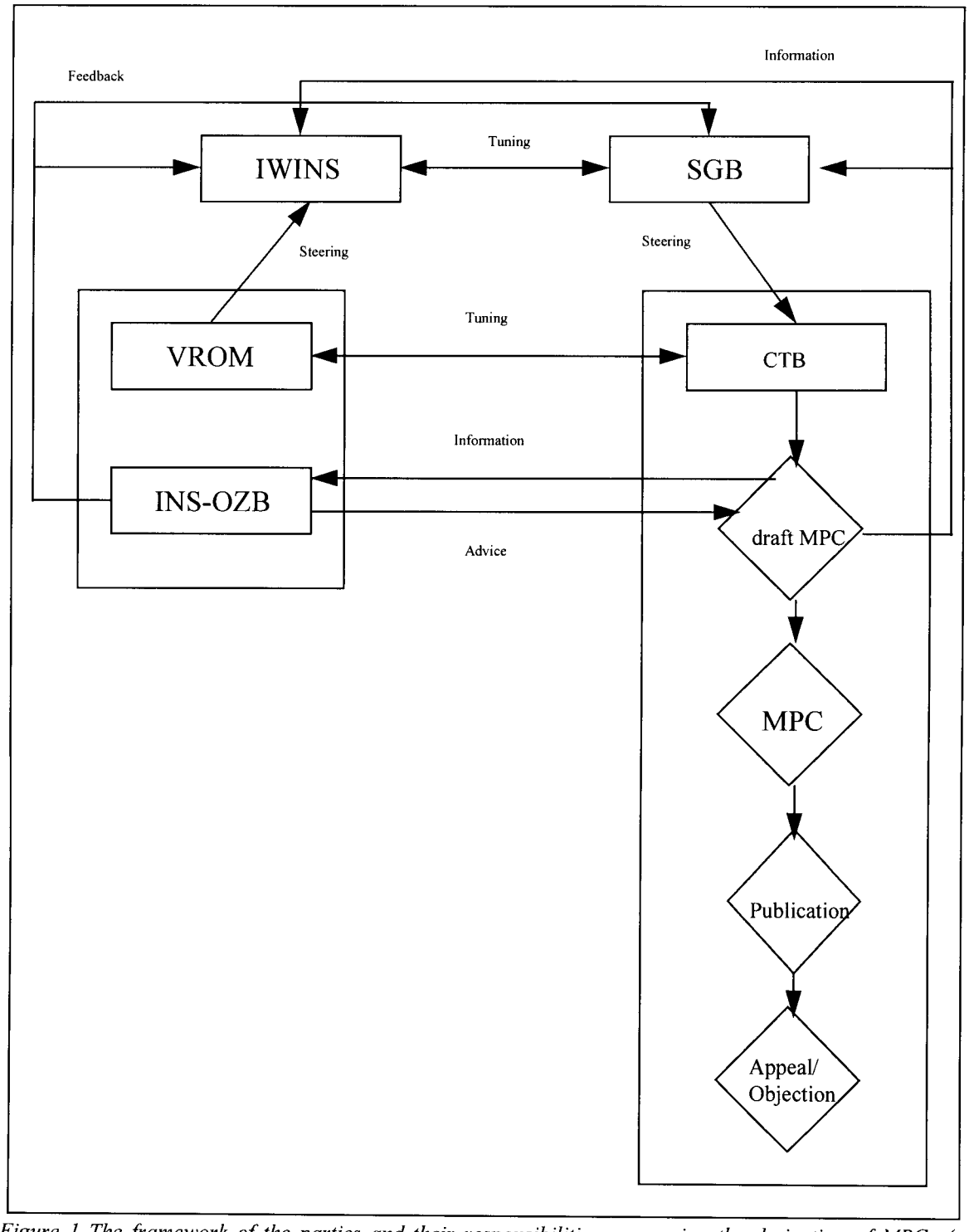

Figure 1 The framework of the parties and their responsibilities concerning the derivation of MPCs (source: ministry of VROM (notition SVS/SN/0536, november 1997).

Table 1 Bottlenecks in the MPC/CTB project

BOTTLENECKS	PROPOSAL	DECISION
1. Assessment factors, what to do and which to choose?	Aldenberg & Slob (1993) and if necessary EU-assessment factors (not modified EPA).	YES
2. Do all three MPCs need to be derived (soil, water and sediment) and do they need to be harmonised?	Yes.	YES
3. How to use the regular registration dossier (admission) and public scientific articles for MPC derivation purposes?	use ecotoxicity endpoints from the registration dossier and the scientific literature; environmental fate endpoints from registration dossiers. $K_{s/l}$ values are derived from Kf, unless the data indicate otherwise (expert judgement). Public literature cannot fill gaps in the admission dossier.	YES, both ecotoxicity and $K_{s/l}$ from Kf
4 Which species to select?	The species selection should be a part of the search profile to ensure a uniform assessment. Efficacy data are used. All data for marine and freshwater species should be combined in principle. Data on all species are included in derivation of MPCs.	YES, all species

Ad 1 Assessment factors used within the different scopes.

MPC values are derived using extrapolation factors. At the moment different sets of extrapolation factors are used in the different scopes.

Setting Integrated Environmental Quality Standards (INS) and Dutch Pesticide Act (CTB)

In the frame INS as well as in the frame CTB (plant protection products and biocides) two complemental extrapolation methods are applied: the refined effects assessment (Aldenberg & Slob, 1993) and the preliminary effects assessment method (modified EPA method). In the latter the following assessment factors are applied:

Table 2 Extrapolation factors used for INS/PPP purposes

Available information	**Assessment factor**
lowest acute L(E)C50-value for acute toxicity	1000
lowest acute L(E)C50-value for acute toxicity for minimal algae/crustacean/fish	100
lowest NOEC-value for chronic toxicity*	10
lowest NOEC-value for chronic toxicity for minimal algae/crustacean/fish	10

*this value is subsequently compared to the extrapolated value based on acute L(E)C50 toxicity values. The lowest one is selected

Biocides

For biocides assessment factors are prescribed that differ from agricultural pesticides: in case of only one long-term NOEC (either fish or water fleas) or two long-term NOECs (fish and/or water fleas and /or algae) the assessment factors should be 100 and 50, respectively (TGD 93/67/EEC, 1488/94, 1996). In table 3 the extrapolation factors for biocides are presented:

Table 3 Extrapolation factors used for biocides

Available information	Assessment factor
at least one short term L(E)C50-value for fish, daphnia and algae	1000
one long term NOEC for fish or daphnia	100
two long term NOEC-values from two trophic levels (fish and/or daphnia and/or algae)	50
three long term NOEC-values from three trophic levels (fish, daphnia and algae)	10
field data or model ecosystems	case by case <10

* for extensive notes on the exact application of the factors see TGD 93/67/EEC, 1488/94 (1996).

Within the frame of the Uniform Principles no MPCs are derived, but a trigger value is derived, by dividing the lowest effect parameter (both acute and chronic, i.e. the test duration) per taxonomic group (fish, algae, daphnids) by an assessment factor. This procedure is also used in the BmB as a first tier assessment. This trigger value is to be compared to a defined exposure value. Because these trigger values are derived per taxonomic group for both acute and chronic exposure, they are not identical to MPCs. The trigger values are only used when data for all three taxonomic groups are available (else no admission is granted because of an incomplete dossier). The lowest trigger value is critical in the admission procedure. Once all dossier requirements are fulfilled, the lowest trigger value does function the way an MPC does. Therefore the use of MPCs is not competely unknown within the frames of the UP and the BmB.

The starting point for this document was to incorporate the methodology used for INS to derive MPCs for pesticides. **However, a problem occurs, *regardless* of the choice made to harmonise both procedures. This problem exceeds the level of competence of CSR/RIVM and decisions should be made by Stuurgroep INS/SGB.**

There are differences in the extrapolation methods applied for plant protection products and INS, and biocides. The result is derivation of different MPCs for substances that are used as biocides, but also have been considered within INS. The solution is to choose one method for all frameworks. As a result all INS-MPCs for pesticides already derived are not based on the harmonised protocol. Using the protocol on the same data set might lead to different MPC values. Besides, harmonising the methodology to accomodate the pesticide registration raises the question whether the INS-MPCs for existing substances should be re-evaluated as well.

It is proposed by CSR to choose for one methodology: the combination of the refined effects assessment (Aldenberg & Slob, 1993) together with the EU-method (TGD 93/67/EEC, 1488/94, 1996). Because the directive on biocides has recently come into force (98/8/EG, 16-2-98, operative since 8-3-98), and the Appendix III of the BmB will be revised in order to accomodate this protocol, the EU-method (TGD 93/67/EEC, 1488/94, 1996), together with the refined effects assessment (Aldenberg & Slob, 1993) is the most logical choice.

The consequences are that existing MPC for pesticides should be re-evaluated in due course of the re-registration by the CTB and that existing MPC for other substances should be re-evaluated after the proposed period of ca. 5 years (i.e. in 2003) (IWINS, 1997). The impact of the new assessment method on the MPCs will be comparable to the impact that new data will have.

Ad 2 Harmonised MPCs?

Should MPCs be harmonised or should MPCs be derived for the individual compartments? In 1997 the involved parties agreed on deriving the MPCs for soil and water, and if necessary for sediment, the moment a product is (re)registered, even when the "unless" criteria of the BmB do not apply (VROM, 1997)[6]. This agreement does not explicitely include that these MPCs should be harmonised. Moreover, the desirability of MPCs for sediment is not fully supported in this letter.

However, the fact that MPC for soil and water, and if necessary for sediment, are to be derived even when the "unless" criteria of the BmB do not apply implies that the desire for the MPC is not related to any specific application, emission or distribution. There is therefore no criterium to determine whether sediment will be relevant or not. Therefore the dilemma of deriving an MPC for sediment or not is no dilemma, because there is no reason to choose between the two alternatives.

Data on toxicity for sediment dwelling species for pesticides or other substances are rare. In INS, for both sediment and soil the equilibrium partitioning method (EP-method) is applied to derive MPCs from MPCs for waterorganisms if not enough data on sediment and soil organisms are available. The EP-method is also used to harmonise the independently derived MPCs for water, soil and sediment.
The consequence of not harmonising MPCs might lead of underestimation of MPCs in one of the other compartments as a result of transport of the chemical based on the compounds physical/chemical properties. Not harmonising also leads to differences in the MPCs for pesticides that are already derived in Crommentuijn *et al.* (1997).

Proposal:
MPCs (for soil, water and sediment) are to be harmonised.

Ad 3 How to use the regular registration dossier and public literature.

INS mainly deals with scientific public literature, the CTB with generally more comprehensive admission dossiers. Therefore, one can say that there are two different types of data. The consequence of using public literature for admission purposes focuses mainly on the reliability and the usefulness of studies. However, it is also important to discuss whether "fate and behaviour" endpoints, mainly sorption, besides toxicity endpoints, should be derived from public literature. Considering all endpoints from public literature may lead to long search actions possibly resulting in disappointing low numbers of useful and reliable studies. Interference with legally embedded deadlines may thus be expected.
Besides this, there are different criteria in INS and the CTB methodology in partition coefficients $K_{s/l}$. The CTB uses the Freundlich isotherm for describing the distribution between the solid and liquid phase (Kf). In INS the experimental data are used for derivation of the partition coefficients in another way[7].
Another question that arises when using public literature is the status of the different literature sources towards registration purposes. The underlying thought behind this question is that if a public literature study is available, and accepted by the CTB, there is no need for the notifier to perform a GLP test according to all the criteria set. However, it is strongly felt that public literature cannot fill gaps in the admission dossier. This feeling is reflected in the fact that the admission assessment does not start until the admission dossier is complete (CTB completeness check).

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[6] Letter of Ir. M. Bovenkerk (VROM/DGM/SVS) to SGB, IWINS and CTB, dd. November 4, 1997, SVS/SN/0536.

[7] The CTB methodology for evaluation of "fate and behaviour" studies is described in more detail in Mensink *et al.* (1995) than for INS in Kalf (1996). The reason is that for admission of pesticides hazard assessment needs to be performed whereas for INS effect assessment must lead to environmental risk limits that are used for estimation of *potential* risks for organisms.

In summary two main questions need to be answered
1) Should other information than toxicity endpoints be derived from public literature?
2) What is the status of public literature versus admission dossier data?

Proposals:
Use ecotoxicity endpoints from the registration dossier and the scientific literature; environmental fate endpoints from registration dossiers[8]. Kp values are derived from Kf, unless the data indicate otherwise (expert judgement). Public literature cannot fill gaps in the admission dossier.

Ad 4 Which species to select?
In the Netherlands Pesticide Act (BMW, 1962) the possibility to exclude species in MPC derivation is written down. This discussion point deals with the questions: what are target species (which definitions and how do we use these species for MPC derivation)?

A target species is defined by RIVM-CSR/CTB as the pest species in the particular system[9].
However, the fact that MPC are to be derived even when the "unless" criteria of the BmB do not apply (VROM, 1997)[10] implies that the desire for the MPC is not related to any specific application, emission or distribution. There is therefore no criterium to determine whether a species is a target species or not, because the use is not yet taken into account. Therefore the dilemma of deriving an MPC with or without target species is no dilemma, because there is no reason to choose between species.

Furhermore, if the use should be taken into account, every use would yield a different MPC. For example, the weed species to be controlled in maize are not the same as in winter cereals. The harmonisation was initiated as to prevent the co-existence of more than one MPC. A solution would be to denote all weeds in all proposed uses as target species, resulting in the highest MPC for the least specific pesticide. The MPC will then be controlled by the manufacturers, that may modify the field of use. The reverse option is to denote all weeds as non-target species, which is in fact has been the strategy of INS all along.

Therefore data on all species should be included in derivation of MPCs. The sensitivity of species within an ecosystem can be described as a distribution function. Generally the reliability of a distribution increases if more input data are available, and overconservative assessment factors are avoided. Efficacy data are used, but because for target species rarely NOEC or EC50 values are available, this will have a relatively low impact on the MPC.

Proposals:
The species selection should be a part of the search profile to ensure a uniform assessment. All data for marine and freshwater species should be combined in principle. Efficacy data are used. Data on all species are included in derivation of MPCs.

[8] Unless the weight of evidence indicates substantial differences between the registration dossier and public literature.
[9] E.g. agro-ecosystem, industrial cooling system; a pesticide used against algae in the industrial cooling system should not kill algae when exposed in the surface water), as described in the "Wettelijk Gebruiksvoorschrift / Gebruiksaanwijzing (WG/GA.
[10] Letter of Ir. M. Bovenkerk (VROM/DGM/SVS) to SGB, IWINS and CTB, dd. November 4, 1997, SVS/SN/0536.

ANNEX 3 GLOSSARY

BCF	BioConcentration Factor: the ratio of the test substance concentration in (part of) an organism (e.g. fish, plant) to the concentration in a medium (e.g. water, soil) at steady state
BmB	Abbreviation in Dutch for "Besluit Milieutoelatingseisen Bestrijdingsmiddelen".
Cb	Background Concentration
CSR	Centrum voor Stoffen en Riscicobeoordeling (Dutch), Centre for Substances and Risk Assessment (English)
CTB	College voor de Toelating van Bestrijdingsmiddelen (Dutch), Board for the Authorisation of Pesticides (English).
DGM	Directoraat-Generaal Milieubeheer (Dutch); Directorate General for Environmental Protection (English)
DT_{50}	time in which 50% of the parent compound has disappeared from soil or water by transformation or degradation (under standard conditions). See degradation and transformation
EC_{50}	median Effective Concentration: 1. the concentration resulting in a 50% change in a parameter (e.g. algal growth) relative to the control 2. the concentration at which a particular effect (e.g. daphnia immobilization) is observed in 50% of the organism population relative to the control
EU	European Union
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice: a set of rules describing how a laboratory should work, how it should be organised and how it can produce valid data; GLP principles are described by e.g. OECD
H	see Henry's Law Constant
Henry's law constant	air-water partition coefficient; the ratio between the partial pressure in the gas phase of a compound and its concentration in water. Henry's law constant can be used with units (Pa/ m^3 / mol^{-1}, synonym is H') or unitless (synonym is H)
IC_{50}	median Inhibitory Concentration: the concentration resulting in a 50% inhibition of growth relative to the control
INS	Abbreviation in Dutch for the project "Setting of Environmental Quality Standards"

IWINS	Abbreviation in Dutch for "Interdepartementale Werkgroep Integrale Normstelling Stoffen", now Stuurgroep INS.
K_{aw}	air-water partition coefficient. See Henry's law constant
K_F	Freundlich coefficient: a soil-water partition coefficient —or sorption coefficient— *dependent* on the exponent 1/n (n is an empirical entity which describes the non-linearity of an adsorption isotherm)
K_{om}	sorption coefficient normalised to the fraction of organic matter in soil
K_{ow}	octanol-water partition coefficient
$K_{s/l}$	soil-water partition coefficient *independent* on the ratio 1/n (n is an empirical entity which describes the non-linearity of an adsorption isotherm)
LC_{50}	median Lethal Concentration: a statistically derived concentration that can be expected to cause death in 50% of animals exposed for a specified time
LD_{50}	median Lethal Dose: statistically derived single dose that can be expected to cause death in 50% of dosed animals
LNV	Ministerie van Landbouw, Natuurbeheer en Visserij (Dutch), Ministry of Agriculture, Nature Management and Fisheries
MJP-G	Abbreviation in Dutch for "Meerjarenplan gewasbescherming"
MPA	Maximum Permissible Addition
MPC	Maximum Permissible Concentration
NOEC	No-Observed-Effect-Concentration: the highest concentration without adverse effects
o.c.	organic carbon
o.m.	organic matter
P	vapour pressure
PAF	Potentially Affected Fraction
partition coefficient	ratio of the distribution of a substance between two phases when the heterogeneous system (of two phases) is in equilibrium; the ratio of concentrations (or, strictly speaking, activities) of the same molecular species in the two phases is constant at constant temperature
PNEC	Predicted NO Effect Concentration
RIVM	Abbreviation in Dutch for the National Institute of Public Health and the Environment

S	Water solubility
SGB	Abbreviation in Dutch for Steering Group Pesticide Policy "Stuurgroep Bestrijdingsmiddelenbeleid"
SVS	Abbreviation in Dutch for "Directie Stoffen, Veiligheid, Straling"
TGD	Technical Guidance Documents
VROM	Abbreviation in Dutch for the Ministry of Housing, Spatial Planning and the Environment

ANNEX 4 APPLICATION OF ASSESSMENT FACTORS TO INS DATA SETS; MODIFIED EPA METHOD VERSUS EU-TECHNICAL GUIDANCE DOCUMENT. RESULTS OF TWO METHODS COMPARED

In INS (Kalf, 1996) the modified EPA is used for derivation of MPC if less than four NOECs for four different species are available. In the harmonised procedure for derivation of MPCs the extrapolation factors of the ECB (1996) presented in the TGD will be applied. The consequences of this change are laid down in RIVM/CSR notice: Van Vlaardingen and van Wezel (1998) CSR report 06416A00; Application of assessment factors to INS data sets; modified EPA method versus EU-Technical Guidance Document. Results of two methods compared. The discussion presented in the mentioned RIVM/CSR notice are repeated below:

Differences between the two methods

Differences between the two methods are discussed in the following:

1. Base set requirement.

EU guidelines demand a minimum of three acute aquatic toxicity tests for a compound to be delivered; the base set. The test organisms should be representative for three different trophic levels i.e. algae, *Daphnia*, fish. To calculate the PNEC, a factor of 1000 is applied to the lowest L(E)C50. Lower assessment factors may be applied if more information is available. Note that lowering of assessment factors is only possible if the base set is complete. Consequently, the assessment stops when the base set is incomplete; a PNEC is not derived. The EU/TGD guidelines allow exceptions to this rule:

- when a compound cannot be tested for acute toxicity testing because of its hydrophobicity (log K_{ow} >3) (EC, 1996, p. 332);
- the TGD states: "There are cases where the base set is not complete (...) In these exceptional cases, the PNEC should be caclulated with a factor of 1000. Variation from a factor of 1000 should not be regarded as normal and should be fully supported by accompanying evidence" (EC, 1996, p. 331). The way this statement is expressed does not allow for a uniform interpretation. For this reason, this exception was not applied in this study.

In MPC derivation for INS purposes, a toxicity-study data set is often less consistent with regard to representation of trophic levels. Its dimension depends on the information as published in public literature. Requirements for risk assessment for the terrestrial compartment are less strict in the EU/TGD framework. A complete base set is not compulsory in this case.

2. Possibilities to lower the assessment factor

In EU/TGD, when assessing the usefulness of long term NOECs, the trophic level of the test species yielding a NOEC is compared to the trophic level of the test species yielding the lowest acute L(E)C50. When the trophic level containing the most sensitive species based on acute toxicity is represented in the chronic toxicity data by a NOEC, the assessment factor may be lowered. Additional NOECs, at different trophic levels, may also lower the assessment factor.

In the modified EPA method, the assessment factor of 1000 can be lowered to 100 if the base-set is complete. This means that minimally one algal-, one crustacean- and one fish L(E)C50 should be available. A comparable rule does exist in the EU/TGD guideline, stating that the assessment factor may be varied (but not be lower than 100) when evidence is present or when a compound is subject to intermittent release. The latter is not applicable to derivation of MPCs. Evidence can be information on structurally similar compounds, mode of action of the compound, toxicity to species covering additional taxonomic groups other than the base set species or toxicity to a

variety of species belonging to the base set taxonomic groups (EC, 1996, p. 330). The latter rule (varying of the assessment factor between 1000 to 100 upon additional evidence) was not applied in the underlying study. It requires thorough interpretation of the referred literature in the reports that are produced until now within the framework of INS which is beyond the scope of this study.

3. Test organisms as representatives of trophic levels.

Acute toxicity.

Within the INS project the following agreements are held with respect to the validity of taxonomic groups as base-set representatives. In acute aquatic toxicity tests, the primary producers should be represented by algal species. Although aquatic macrophyta are primary producers as well, they are considered to be a separate group ('higher plants') and as such they are not valid representatives when base-set (acute toxicity) completeness is demanded. Neither are macrophyte data accepted to replace algal studies, when these are absent. The trophic level of primary consumers should at least be represented by a crustacean species, as opposed to the EU/TGD guideline where a *Daphnia* test result is required. This requirement is rather strict when applied to data sets obtained from public literature. The level of secondary consumers should be represented by a fish species in both methods.

Chronic toxicity.

Within the framework of INS, in the chronic toxicity data set macrophyta are considered to be part of the trophic level of primary producers. As mentioned before, chronic macrophyte data (NOECs) are not accepted as representative for the primary producers when no data on algae are present. If a macrophyte study is the only study present, its result may be used for the risk assessment. Within the group of primary consumers, all annelids, molluscs, arthropods etc. are accepted as valid contributors to the chronic (NOEC) data set. Fishes constitute the level of secondary consumers.

In contrast, the EU/TGD demands chronic data on fish, and/or *Daphnia* and/or algae. Therefore, if no toxicity data on *Daphnia* are available in public literature, a higher assessment factor should be used whereas in the INS project, toxicity data on other representatives of the trophic level of primary consumers may be used. For this study we have applied the TGD as it is written, i.e. strictly. However, literally reading the TGD may exclude many valuable toxicity studies from the risk assessment.

4. Calculation of the mean of more toxicity studies on one organism

In the EU/TGD it is stated that if more than one L(E)C50 or NOEC is available, and it is concluded that variation in response is not due to differences in test conditions, the arithmetic mean of the effect concentrations is calculated and subsequently used in the risk assessment. This differs from the procedure followed within the INS framework: the geometric mean is used in this case.

Expert judgement

Both the modified EPA method and the EU/TGD method leave room for adjustment of the assessment factors based on expert judgement (see also section 0-2) In those cases where the use of expert judgement was clarified in INS reports, conclusions were taken over indiscriminately in this study, in order not to obscure the comparison of the assessment methods. An example of expert judgement application is given by organophosphorous-insectide toxicity. In data sets on organophosphorous-insecticide toxicity to aquatic organisms, little data were available on toxicity to algae. Since these compounds act as choline-esterase inhibitors, it was argued that algae would be less sensitive than insects and crustaceans; which was confirmed in those cases where data were available. It was decided that for those cases where data on algae were lacking while data on insects and crustaceans were present, an assessment factor of 100 instead of 1000 was used in the assessment.

When a protocol for MPC derivation for the harmonized procedure will be written, it is recommended to include explicitly where expert judgment is allowed within the EU/TGD method. At least hydrophobicity (see section 0-1:

"Base set requirement") and additional evidence (see 0-2: "Possibilities to lower the assessment factor") should be inlcuded.

Secondary poisoning

There are four priority compounds for which an MPC for secondary poisoning currently exists: pentachlorophenol, α-HCH, β-HCH and γ-HCH (IWINS, 1997). Within the framework of the INS project, MPCs for secondary poisoning have been derived (Van de Plassche, 1994). After advices of the Dutch Health Council and the Technical Soil Protection Committee, a different approach was used, resulting in the MPCs as listed in the IWINS report (IWINS, 1997). Since the procedure underlying the derivation of the existing values is unknown, alternative values MPC values cannot be derived.

There is a difference however in application of assessment factors between the modified EPA method and the EU/TGD. For reasons of completeness we give the rules for the use of assessment factors when extrapolating bird and mammal toxicity data for both methods.

EU/TGD (ECB, 1996, p. 350-351):

- Acute LD50 studies on rats or birds are not extrapolated to a chronic value
- Acute avian dietary (5 days) LC50 values are extrapolated using a factor of **1000**
- NOEC from 28 day repeated dose test: a factor of **100** is applied to the NOEC
- NOEC from 90 day toxicity test: a factor of **30** may be applied
- NOEC form chronic studies are available: a factor of **10** may be applied
- NOEC reproduction studies: a factor of **10** may be applied.

INS/modified EPA method (Van de Plassche, 1994):

Table 5.1. modified EPA method for extrapolation of results from of bird and mammal studies.

Available information	**Assessment factor**
less than 3 acute LC50-valuesfrom different taxonomic groups and no chronic NOECs	1000
at least 3 acute LC50-valuesfrom different taxonomic groups and no chronic NOECs	100
less than 3 chronic NOECs from different taxonomic groups	10
3 chronic NOECs from different taxonomic groups	10

*this value is subsequently compared to the extrapolated value based on acute LC50 toxicity values. The lowest one is selected

Conclusions

The rules for the application of the EU/TGD method to toxicity data are more strict than those of the modified EPA method. The most stringent rule is that for the aquatic compartment, completeness of the base set is demanded. If no acute toxicity data on algae, *Daphnia* and fish are available a risk assessment is not performed, unless the log K_{ow} of a compound is >3. In that case, base set completeness is no longer required, but chronic data should then be available. In INS practice, i.e. applying these rules to data sets obtained from literature, for many compounds too few data are available to allow application of an assessment factor.

In this document, the application of the assessment method according to the EU/TGD guidelines was performed only for priority compounds. For many of these compounds, MPCs have not been derived. For other compounds MPCs exist, but these were derived using other methods than the modified EPA method. A comparison of these MPCs with MPCs derived using the EU/TGD method would be useless and is therefore not performed.

Of the 19 MPCs calculated for this report using the EU/TGD method, 2 were higher than the existing MPC (derived in INS), 13 were lower and 4 did not alter. For priority compounds that currently exceed the Dutch quality standards and for which the risk assessment underlying the MPC is conservative due to limited availability

of toxicity data, generating additional toxicity data may be more cost-effective than carrying out measures of control.

Summarizing, we can say that the strictness of the EU/TGD rules leads to a decrease of the number of MPCs that can be derived. This may imply that toxicity data should be generated when a literature search on recent years does not yield additional information. Otherwise, the modified EPA method may still be used. In a follow-up study alternative MPCs could be derived for all compounds for which an MPC currently exists.

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ANNEX 5 REFERENCE LINES DERIVED FROM CROMMENTUIJN *ET AL.* (1997B), TABLE 5.1 PAGE 62)

Table 5.1 For soil and sediment the reference line is given which is used to calculate the background concentrations in soil/sediment (L= % clay; H= % organic matter): C*b*(soil/sed), values are expressed as a concentration in standard soil (soil containing 10% organic matter and 25%).

metal	Reference line	C*b*(soil/sed) total (mg/kg)
antimony	3.0 (d)	3.0 (b)
arsenic	15 + 0.4 (L + H) (a)	29(a)
barium	30 + 5L (d)	155(b)
beryllium	0.3 + 0.033L (d)	1.1 (b)
cadmium	0.4 + 0.007 (L + 3H) (a)	0.8 (a)
chromium	50 + 2L (a)	100 (a)
cobalt	2 + 0.28 L (d)	9.0 (b)
copper	15 + 0.6 (L + H) (a)	36 (a)
lead	50 + L + H (a)	85 (a)
mercury	0.2 + 0.0017 (2L + H) (a)	0.3 (a)
molybdenum	0.5 (d)	0.5 (b)
nickel	10 + L (a)	35 (a)
selenium	0.7 (d)	0.7 (b)
thallium	-	1.0 (b)*
tin	4+ 0.6L (d)	19 (b)
vanadium	12 + 1.2L (d)	42 (b)
zinc	50 + 1.5 (2L + H) (a)	140 (a)

Notes:

(a): Van den Hoop (1995a),

(b): Van de Plassche and De Bruijn (1992),

(c): Calculated using equation 9,

(d): De Bruijn and Denneman (1992),

*: adjusted on the basis of the advise of the Technical Soil Protection Committee (TCB, 1994).

ANNEX 6 AN ALTERNATIVE METHOD FOR INCORPORATING SECONDARY POISONING.

Secondary poisoning is concerned with toxic effects in the higher members of the food chain which result from ingestion of organisms at the different trophic levels that contain accumulated substances.
Bioconcentration is the net result of uptake, distribution and elimination of a substance in an organisms due to water-borne exposure, whereas bioaccumulation includes all routes, i.e. air, water, soil and food. Biomagnification is the accumulation and transfer of chemicals via the food chain, resulting in an increase of the internal concentration in organisms at the higher levels in the trophic chain.

Two aquatic food chains (water → fish → fish-eating predators and water → mussel → mussel-eating predators) and one terrestrial food chain (soil → earthworm → worm-eating predators) are considered. Two methods are available for incorporating secondary poisoning (Van de Plassche, 1994):

- in method 1 data sets for lower organisms (i.e. fresh- and saltwater organisms for the aquatic food chain and soil organisms of the terrestrial food chain) and top predators (i.e. birds and mammals) are treated separately. Two MPCs are calculated from which one is selected.
- in method 2 both data sets are combined: first all individual NOECs for birds and mammals are divided by the BCF to obtain concentrations in water or soil. These values are used as input data for the TGD method or the statistical extrapolation method of Aldenberg and Slob together with the L(E)C50 or NOEC values for aquatic or soil organisms. This method is dealt with in the main document.

For method 1 the following algorithm was proposed by Romijn *et al.* (1993):

Equation 6-1: Algorithms to calculate the MPC for secondary poisoning

$$MPCwater = NEC_{bird;mammal} / BCF_{fish}$$
$$MPCsoil = NEC_{bird;mammal} / BCF_{worm}$$

The $NEC_{bird;mammal}$ can be considered as a maximum concentration in food which will not lead to adverse effects after ingestion of this food. The NEC is based on toxicity data for predators like birds and mammals. Preferably, this should be data for fish-eating birds and mammals. However, these data are seldomly available. Therefore, data on other bird and mammalian species, exposed via the food, have to be used.

Toxicity data for birds and mammals result in LC50 (e.g. 5 days dietary study with birds) or NEC values (e.g. 28 days oral study with rats). If results are expressed in mg/kg body weight they should be converted to mg/kg food using conversion factors. In the EU Technical Guidance Document the following factors are proposed:

Table 6-1: Conversion factors for recalculation of body weight concentrations to concentrations in food; birds and mammals (ECB, 1996)

Species	**Conversion factor**
Canis domesticus:	40
Macaca spec.:	20
Microtus spec.:	8.3
Mus musculus:	8.3
Oryctolagus cuniculus:	33.3
Rattus norvegicus > 6 weeks old:	20
Rattus norvegicus < 6 weeks old:	10

Extrapolation from these LC50 and NOEC values gives the NEC. Assessment factors have to be used which take into account interspecies variation, subchronic to chronic toxicity extrapolation and laboratory to field impact extrapolation. In the Technical Guidance Document (ECB, 1996) the following assessment factors are used:

Table 6-2: Assessment factors for extrapolation of bird and mammal data according to the TGD

Information	**Assessment factor**
BIRDS	1000
5 days avian dietary LC50	
MAMMALS	100
28 days test	
90 days test	30
chronic study	10

BCF is short for Bioconcentration Factor. The BCF can be measured or calculated. The static BCF is the ratio between the concentration in the organism and the concentration in a steady-state (sometimes also called equilibrium) situation. When uptake (k_1) and depuration (k_2) kinetics are measured, the dynamic BCF can be calculated from the quotient of the uptake and depuration rate constants.

Equation 6-2: Calculation of the BCF from the quotient of the uptake and depuration rate constants.

$$BCF = C_{organisms} / C_{water} \text{ or } k_1 / k_2$$

A geometric mean is calculated from the BCF values available. If more than one value is available on a single species a geometric mean is calculated first, before an overall geometric mean is calculated.

If measured BCF values are not available the BCF can be predicted from the relationship between the K_{ow} and BCF. The following relationships are used for fish and mussels:

Equation 6-3 and 6-4: Calculation of the BCF from the log K_{OW}

$$BCF_{fish} \text{ (whole body, fresh weight)} = 0.05 * K_{OW}$$

$$BCF_{mussel} \text{ (whole body, fresh weight)} = 0.013 * K_{OW}$$

For organic compounds a BCF for worms of 10 kg/kg is used. For metals experimentally determined BCFs for earthworms are used.

Based on the work of Romijn *et al.* (1993), Everts *et al.* (1993) discussed whether so called correction factors should be applied for several aspects which influence secondary poisoning:

- laboratory - field conversion: differences in metabolic rate between animals in laboratory (toxicity tests) and the field;
- caloric conversion: differences in caloric content of the different types of food: cereals versus fish, mussels or earthworms;
- normal versus extreme conditions: differences in metabolic rate under normal field conditions and more extreme ones like breeding period, migration and winter;
- food assimilation efficiency: differences in use of different types of food;
- pollutant assimilation efficiency: differences in bioavailability in test animals (surface application of a test compound) and in the field (compound incorporated in food);
- relative sensitivity: differences in biotransformation of certain compounds between taxonomic groups of birds or mammals.

Values for several correction factors are proposed by Traas *et al.* (in press). Of these factors the one for caloric conversion has a firmer scientific basis than the other ones (Dutch Health Council, 1993). This factor is based on an extensive literature search on differences in caloric content between laboratory food versus fish and mussels. Subsequently, this leads to the following adaptation of equation 6-1:

Equation 6-5 and 6-6: Calculation of MPCs using caloric conversions

$$MPC_{water} = NEC_{bird;mammal} \times 0.32 / BCF_{fish}$$

$$MPC_{water} = NEC_{bird;mammal} \times 0.20 / BCF_{mussel}$$

Because mussels have a lower caloric value than fish the correction factor is higher. Predators must consume more mussels compared to fish to obtain the same amount of energy. On the other hand the BCF for most fish is higher than the one for mussels.

In the same project as mentioned above a correction factor of 0.23 is derived for earthworms based on Westerterp *et al.* (1982) It should be stated that this correction factor is based on a limited data-set compared to the one for mussels and fish.

Equation 6-7: Calculation of MPCs using caloric conversions

$$MPC_{soil} = NEC_{bird;mammal} \times 0.23 / BCF_{worm}$$

ANNEX 7 ASSESSMENT FACTORS ACCORDING TO THE TECHNICAL GUIDANCE DOCUMENT (ECB, 1996).

The chapters in the TGD concerning the assessment factors for the aquatic, sediment and terrestrial ecosystem are reprinted below. References in the text are not incorporated in the list of literature for the main document. References to annexes do not refer to the annexes of the main report. Formulas concerning the indirect method are omitted. The numbering of tables has no relation to the numbering in the main document.

EFFECTS ASSESSMENT FOR THE AQUATIC COMPARTME NT

Calculation of PNEC

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

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

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

For all new substances the pool of data from which to predict ecosystem effects is very limited: only short-term data are available at the base-set. For most existing substances the situation is the same: in many cases, only short-term toxicity data are available. In these circumstances, it is recognised that, while not having a strong scientific validity, empirically derived assessment factors must be used. Assessment factors have also been proposed by the EPA and OECD (OECD, 1992d). In applying such factors, the intention is to predict a concentration below which an unacceptable effect will most likely not occur. It is not intended to be a level below which the chemical is considered to be safe. However, again, it is likely that an unacepptable effect will not occur.

In establishing the size of these assessment factors, a number of uncertainties must be addressed to extrapolate from single-species laboratory data to a multi-species ecosystem. These areas have been adequately discussed in other papers, and may best be summarised under the following headings:

- Intra- and inter-laboratory variation of toxicity data.
- Intra- and inter-species variations (biological variance).
- Short-term to long-term toxicity extrapolation.
- Laboratory data to field impact extrapolation.

(Extrapolation is required from mono-species tests to ecosystem. Additive, synergistic and antagonistic effects arising from the presence of other substances may also play a role).

The size of the assessment factor depends on the confidence with which a $PNEC_{water}$ can be derived from the available data. This confidence increases, if data are available on the toxicity to organisms at a number of trophic levels, taxonomic groups and with lifestyles representing various feeding strategies. Thus lower assessment factors can be used with larger and more relevant data-sets than the base-set data. The proposed assessment factors are presented in 2.

For new substances an assessment factor of 1000 will be applied on the lowest L(E)C50 of the base-set. Also for existing substances the assessment factor is generally applied to the lowest of the relevant available toxicity data, irrespective of whether the species tested is a standard organism (see notes to 2). For short-term tests, the $L(E)C_{50}$ is used, while the NOEC is used with long-term tests. For some compounds, a large number of validated short-term $L(E)C_{50}$ values may be available. Therefore, it is proposed to calculate the arithmetic mean if more than one $L(E)C_{50}$ value is available for the same species. Prior to calculating the arithmetic mean an analysis of test conditions has to be done in order to find out why differences in response were found.

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

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

Table 2 *Assessment factors to derive a PNEC*

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

NOTES:

(a) The use of a factor of 1000 on short-term toxicity data is a conservative and protective factor and is designed to ensure that substances with the potential to cause adverse effects are identified in the effects assessment. It assumes that each of the above identified uncertainties makes a significant contribution to the overall uncertainty.

For any given substance there may be evidence that this is not so, or that one particular component of the uncertainty is more important than any other. In these circumstances it may be necessary to vary this factor. This variation may lead to a raised or lowered assessment factor depending on the evidence available. Except for substances with intermittent release (see section **Error! Reference source not found.**) under no circumstances should a factor lower than 100 be used in deriving a $PNEC_{water}$ from short-term toxicity data.

Evidence for varying the assessment factor could include one or more of the following:

- Evidence from structurally similar compounds (Evidence from a closely related compound may demonstrate that a higher or lower factor may be appropriate).

- Knowledge of the mode of action. (Some substances, by virtue of their structure, may be known to act in a non-specific manner. A lower factor may therefore be considered. Equally a known specific mode of action may lead to a raised factor).
- The availability of data from a wide selection of species covering additional taxonomic groups other than those represented by the base-set species.
- The availability of data from a variety of species covering the taxonomic groups of the base-set species across at least three trophic levels.

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

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

Variation from a factor of 1000 should not be regarded as normal and should be fully supported by accompanying evidence.

(b) An assessment factor of 100 applies to a single long-term NOEC (fish or Daphnia) if this NOEC was generated for the trophic level showing the lowest $L(E)C_{50}$ in the short-term tests.

If the only available long-term NOEC is from a species (standard or non-standard organism) which does not have the lowest $L(E)C_{50}$ from the short term-tests, it cannot be regarded as protective of other more sensitive species using the assessment factors available. Thus the effects assessment is based on the short-term data with an assessment factor of 1000. However, the resulting PNEC based on short-term data may not be higher than the PNEC based on the long-term NOEC available.

An assessment factor of 100 applies also to the lowest of two long-term NOECs covering two trophic levels when such NOECs have not been generated from that showing the lowest $L(E)C_{50}$ of the short-term tests.

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

(d) An assessment factor of 10 will normally only be applied when long-term toxicity NOECs are available from at least three species across three trophic levels (e.g. fish, Daphnia, and algae or a non-standard organism instead of a standard organism).

When examining the results of long-term toxicity studies, the $PNEC_{water}$ should be calculated from the lowest available no observed effect concentration (NOEC). Extrapolation to the ecosystem effects can be made with much greater confidence, and thus a reduction of the assessment factor to 10 is possible. This is only sufficient, however, if the species tested can be considered to represent one of the more sensitive groups. This would normally only be possible to determine if data were available on at least three species across three trophic levels. It may sometimes be possible to determine with high probability that the most sensitive species has been examined, i.e. that a further long-term NOEC from a different taxonomic group would not be lower than the data already available. In those circumstances, a factor of 10 applied to the lowest NOEC from only two species would also be appropriate. This is particularly important if the substance does not have a potential to bioaccumulate. If it is not possible to make this judgement, then an assessment factor of 50 should be applied to take into account any interspecies variation in sensitivity.

A factor of 10 cannot be decreased on the basis of laboratory studies.

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

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

(g) For substances for which no toxicity is observed in short term tests a long term test has to be carried out if the log Kow > 3 (or BCF > 100) and if the $PEC_{local/regional}$ is > 1/100th of the water solubility (see section **Error! Reference source not found.**). The long-term toxicity test should normally be a Daphnia test to avoid unnecessary vertebrate testing. The NOEC from this test can then be used with an assessment factor of 100. If in addition to the required long-term test a NOEC is determined from an algae test of the base-set an assessment factor of 50 is applied.

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

Effects assessment for substances with intermittent release

For substances subject to intermittent release (see section **Error! Reference source not found.** for the definition of intermittent release), exposure may be of only short duration. At least for dynamic systems like rivers the likelihood of long-term effects arising from such exposure is low, the principal risk being short-term toxicity effects. In extrapolating to a $PNEC_{water}$, therefore, generally only short-term effects need to be considered. It is therefore proposed that normally an assessment factor of 100 be applied to the lowest $L(E)C_{50}$ of at least three short-term tests from three trophic levels to derive a $PNEC_{water}$ for such situations. The assessment factor is used to allow the extrapolation from the short-term toxicity laboratory test to short-term effects in ecosystems. In undertaking such an extrapolation, due account is taken of the biological variables of intra- and inter-species toxicity, as well as the general uncertainties in predicting ecosystem effects from laboratory data.
This extrapolation should be carried out with care. Some substances may be taken up rapidly by the aquatic organism which can lead to delayed effects even after emission has stopped. This will generally be taken into account by the assessment factor of 100 but there may be occasions when a higher or lower factor would be appropriate. For substances with a potential to bioaccumulate the lowered assessment factor of 100 may not always be justified.
For substances with a known non-specific mode of action, inter-species variations may be low. In such cases, a lower factor may be appropriate. In no case should a factor lower than 10 be applied to a short-term $L(E)C_{50}$ value.

Effects assessment for micro-organisms in a STP

As chemicals may cause adverse effects on microbial activity in STPs it is necessary to derive a $PNEC_{micro\text{-}organisms}$ (see section **Error! Reference source not found.**). The $PNEC_{micro\text{-}organisms}$ will be used for the calculation of the PEC/PNEC ratio concerning microbial activity in STPs. Current test systems for measuring the impact of chemicals on microbial activity have different endpoints and sensitivities. At present, only a few internationally accepted test systems, such as OECD 209 (inhibition of respiration of activated sludge) and ISO 9509 (inhibition of nitrification) exist. Available data (e.g. Umweltbundesamt, 1993; Reynolds et al., 1987) suggest the following range of increasing sensitivities: respiration inhibition test (OECD 209) < inhibition control in base-set tests < growth inhibition test with *P. putida* < inhibition of nitrification.
Generally, short-term measurements in terms of hours (e.g. 10 h) are preferred, in accordance with the retention time in a STP. Also the information available on the toxicity for micro-organisms has to be relevant for the endpoint considered, i.e. microbial degradation acitivity in a STP. It is clear that test systems like the respiration inhibition test and inhibition of nitrification test can be used. Respiration tests using a mixed inoculum are considered more relevant than respiration inhibition tests using another inoculum. Often also information may be present on individual

bacterial population like MICROTOX, Pseudomonas putida, Pseudomonas fluorescens and even Escherichia coli. These tests must be considered as less relevant. The tests with P. fluorescens and E. coli (Bringmann and Kühn, 1960) cannot be used for determination of the $PNEC_{micro\text{-}organisms}$ as they use glucose as substrate. Also the MICROTOX test cannot be used as a saltwater species is tested. Results of the cell multiplication inhibition test with P. putida (Bringmann and Kühn, 1980) can be used but should be treated with care.
For assessing the toxicity for a substance to micro-organisms in a STP, the effluent concentration will be compared to microbial effect data. A $PNEC_{micro\text{-}organisms}$ is derived as follows:

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

EFFECTS ASSESSMENT FOR THE SEDIMENT

Introduction

Sediments may act as a sink for, and source of chemicals (through resuspension), through sorption of chemical contaminants to particulate matter. Sediments integrate the effects of surface water contamination over time and space, and may thus present a hazard to aquatic communities (both pelagic and benthic) which is not directly predictable from concentrations in the water column. Effects on benthic organisms are of concern because in many habitats the sediment plays an important role in the recycling of detrital material.
No data for sediment dwelling organisms will be available for new substances. To date, only few tests for sediment organisms have been conducted in Europe with existing substances. Research is in progress in this field in various countries however. The selection of representative organisms and the selection of standardised sediments are still being discussed. Various approaches (e.g. equilibrium partitioning, interstitial water quality, spiked sediment toxicity, tissue residue, derived sediment quality criteria and standards) are being developed to investigate the effects chemicals have on sediment and sediment organisms (OECD, 1992b). When standardised tests have been conducted and the assessment factors agreed upon, the calculated $PNEC_{sed}$ can be compared with the estimated concentration in the sediment (PEC_{sed}) or with the concentration of the chemical measured in the sediment. Test procedures are described in ASTM (1990 a-e), ASTM (1991) and Burton (1991 and 1992). In addition OECD is preparing a detailed review paper on aquatic ecotoxicity tests including sediment test methods (Water Quality Institute and RIVM, final draft 1995). In Appendix VI sediment toxicity tests are listed which are used in the United States (Burton, 1991).

Calculation of PNEC

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

- Sediment-dwelling organisms and water column organisms are equally sensitive to the chemical.
- Concentration in sediment, interstitial water and benthic organisms are at thermodynamic equilibrium: the concentration in any of these phases can be predicted using the appropriate partition coefficients.
- Sediment/water partition coefficients can either be measured or derived on the basis of a generic partition method from separately measurable characteristics of the sediment and the properties of the chemical. (For the

derivation of the sediment-water partition coefficient and the limits of the calculation methods see section **Error! Reference source not found.**).

Regardless of whether the Kp_{sed} is measured or estimated, the following remark has to be made for the calculation of $PNEC_{sed}$ using the equilibrium partitioning method. The formula only considers uptake via the water phase. However, uptake may also occur via ingestion of sediment. This may become important, especially for adsorbing chemicals, for example those with a log Kow greater than 3 (equivalent to a calculated Kp_{sed} of 20 with a Foc of 5%). Thus, for these compounds the total uptake may be underestimated. There is evidence from studies in soil (Belfroid et al., 1995), that the proportion of the total dose remains low for chemicals with a log Kow up to 5. Although it is recognised that in principle results for the soil compartment may not be extrapolated to the sediment compartment, it is considered that the possible underestimation of exposure is acceptable when using the equilibrium partitioning method for chemicals with a log Kow between 3 and 5. For compounds with a log Kow greater than 5 (equivalent to a calculated Kp_{sed} of 2000 with a Foc of 5%) the equilibrium method is used in a modified way. In order to take uptake via ingestion of sediment into account, the PEC_{sed} is increased by a factor of 10 for these compounds. It should be kept in mind that this approach is considered as a screening for assessment of the risk to sediment dwelling organisms. The assessment approach described here should be developed further in the future.

When no measured data on sediment and sediment organisms are available, the assessment conducted on the aquatic compartment will also cover the sediment for chemicals with a log Kow up to 5. If a measured bulk concentration in sediment is available, the formula can be applied and the $PNEC_{sed}$ compared with the measured concentration. This will be the normal situation but other situations may also occur. In 3 an overview is given of all possibilities and how to carry out the assessment. The table presents different data configurations and it explains how to use them for the risk characterisation for sediment. If no measured data are available, either for the determination of PEC_{sed} nor for the calculation of $PNEC_{sed}$, no quantitative risk characterisation for sediment can be performed.

***Table 3**: Requirements for performing a risk characterisation for sediment*

Available measured data: PEC_{sed}	**Available measured data: $PNEC_{sed}$**	**Risk characterisation**
$C_{pore\ water}$	none	$\frac{C_{pore\ water}}{PNEC_{water}}$
C_{bulk}	none	$\frac{C_{bulk}.RHO_{sed}.103}{K_{sed\text{-}water}.PNEC_{water}}$
none	$PNEC_{sed}$	$\frac{K_{sed\text{-}water}.PEC_{water}}{PNEC_{sed}.RHO_{sed}.103}$
$C_{pore\ water}$	$PNEC_{sed}$	$\frac{K_{sed\text{-}water}.C_{pore\ water}}{PNEC_{sed}.RHO_{sed}.103}$
C_{bulk}	$PNEC_{sed}$	$\frac{C_{bulk}}{PNEC_{sed}}$
where: $C_{pore\ water}$ concentration in sediment pore water [mg.l-1] C_{bulk} concentration in whole sediment [mg.kg_{sed}-1]		

Available measured data: PEC_{sed}	**Available measured data: $PNEC_{sed}$**	**Risk characterisation**
$K_{sed\text{-}water}$	sediment-water partitioning coefficient [m3.m-3]	eq. **Error! Bookmark not defined.**
RHO_{sed}	density of moistened sediment [kg.m-3]	eq. **Error! Bookmark not defined.**

Effects assessment for the terrestrial compartment

Introduction

Chemicals can reach the soil via several routes: application of sewage sludge in agriculture, direct application of chemicals and deposition from the atmosphere. This means that the possibility of adverse effects has to be assessed. The proposed strategy in this section is based on effects of chemicals on soil organisms. At the moment no strategy is available to assess possible effects on soil functions like filtration, buffering capacity and metabolic capacity.
As mentioned in the introduction, the substances discharged into the soil can not only affect the soil organisms but can influence soil functions. Substances that are hydrophilic and that are readily eluted with the rain water into the ground water as well as those that geoaccumulate and those that are poorly degradable in soil should be considered with special care.
The terrestrial ecosystem comprises both an above-ground community, a soil community and a groundwater community. In this section only effects on soil organisms exposed directly via pore water and/or soil are adressed. It is recognized that the strategy described here must therefore be regarded as a provisional one. However, reference is made to the strategy for the compartment air (section **Error! Reference source not found.**) and for bioaccumulation and secondary poisoning of birds and mammals (section **Error! Reference source not found.**). So far, it is not possible to carry out effect assessment for the groundwater community because no toxicity data are available. Ecotoxicity tests with groundwater fauna and microflora have been proposed by Notenboom and Boessenkool (1992) and Van Beelen et al. (1990).

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

Strategy for effects assessment for soil organisms

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

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

- if no toxicity data are available for soil organisms, the equilibrium partitioning method is applied to identify a potential risk to soil organisms. This method is regarded as a "screening approach" and is explained in section **Error! Reference source not found.** (see also section **Error! Reference source not found.** sediment).
- if toxicity data are available for a producer, a consumer and/or a decomposer the $PNEC_{soil}$ is calculated using assessment factors. The assessment factors are presented in section **Error! Reference source not found.**.
- if only one test result with soil dwelling organisms is available the risk assessment is performed both on the basis of this test using assessment factors and on the basis of the equilibrium partition method. From both $PEC_{soil}/PNEC_{soil}$ ratios the highest one is chosen for the risk characterisation.

The applicability of the equilibrium partitioning method has been tested less for soil than for sediment-dwelling organisms. Van Gestel and Ma (1993) have shown the model to be valid for short term toxicity of several chlorophenols, chlorobenzenes and chloroanilines to earthworms. As for sediment the equilibrium partitioning method may not be suitable for lipophilic compounds and species that are exposed primarily through food (Van

Gestel, 1992). Therefore the same approach is used as for the derivation of the $PNEC_{sediment}$: in order to take uptake via ingestion of soil into account the PEC_{soil} is increased by a factor of 10 for compounds with a log Kow > 5.

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

Calculation of PNEC using assessment factors

The same assessment factors are used for the terrestrial system (see 4) as for the aquatic system (see 2) depending on the type of investigations (short-term or long-term toxicity test), the number of trophic levels tested and the general uncertainties in predicting ecosystem effects from laboratory data. The suggested assessment factors for the soil compartment are not based on comprehensive experience. As already stated information from tests with soil organisms will only be available for some compounds. Also, in most cases this will be information from short-term tests with earthworms. This means that a deeper understanding of the difference between short- and long-term toxicity for several taxonomic groups and the difference between laboratory and field tests is needed. Also the choice of taxonomic groups for which toxicity data are necessary (conform the base-set of algae, Daphnia and fish for the aquatic environment), is a point of discussion. A data-set consisting of toxicity data for primary producers, consumers and decomposers is preferred. However, an internationally accepted set of standardized ecotoxicological tests for hazard assessment of chemicals for the soil compartment is not available at the moment. Reference can be made to section **Error! Reference source not found.** and an OECD project in which a testing strategy for terrestrial ecosystems is being developed (Léon and Van Gestel, 1994). Summarizing, the assessment factors proposed in 4 must be regarded as indicative factors. As more information on the sensitivity of soil organisms becomes available these factors may have to be adjusted.

Table 4 *Assessment factors to derive a PNEC*

Information available	**Assessment factor**
$L(E)C_{50}$ short-term toxicity tests (e.g. plants, earthworms, or micro-organisms)	1000
NOEC for one long-term toxicity test (e.g. plants)	100
NOEC for additional long-term toxicity tests of two trophic levels	50
NOEC for additional long-term toxicity tests for three species of three trophic levels	10
Field data/data of model ecosystems	case-by-case

The $PNEC_{soil}$ is calculated on the basis of the lowest effect value measured. If short-term tests with a producer, a consumer and/or a decomposer are available, the test result is divided by a factor of 1000 to calculate the $PNEC_{soil}$. If only one terrestrial test is available (earthworms or plants), the risk assessment should be performed both on the basis of this terrestrial test and on the basis of the aquatic toxicity data as an indication of the risk to soil organisms. As a precaution, the larger $PEC_{soil}/PNEC_{soil}$ ratio determines which further actions should be taken in the framework of the further testing strategy. The other factors listed in 4 are applied, if more tests than the short-term toxicity test have been conducted.