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Guidance for the derivation of environmental risk limits within the framework of 'International and national environmental quality standards for substances in the Netherlands' (INS)

Revision 2007

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This report is based on:

Lepper P. 2005. Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC). Schmallenberg, Germany: Fraunhofer-Institute Molecular Biology and Applied Ecology. **Version dated September 15, 2005.**

European Commission. 2003. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. Ispra, Italy: European Chemicals Bureau, Institute for Health and Consumer Protection.

Rapport in het kort

Handleiding voor de afleiding van milieurisicogrenzen binnen het raamwerk '(Inter)nationale Normen Stoffen' (INS) - Revisie 2007

Dit rapport is de handleiding voor het afleiden van milieurisicogrenzen die worden gebruikt in het Nederlandse milieubeleid. Het rapport is een herziening van de INS-handleiding uit 2001. Nederland onderscheidt vier milieurisicogrenzen: het verwaarloosbaar risiconiveau (VR), het maximaal toelaatbaar risiconiveau (MTR), het ernstig risiconiveau (ER) en de maximaal toelaatbare concentratie voor ecosystemen (MAC_{eco}).

Welke basisgegevens zijn nodig voor het afleiden van een milieurisicogrens? De handleiding geeft dit overzicht en beschrijft hoe deze literatuurgegevens moeten worden geëvalueerd op juistheid en bruikbaarheid. Vervolgens wordt de methodiek voor het afleiden van milieurisicogrenzen beschreven, inclusief de benodigde berekeningen. Voor water en sediment is deze gelijk aan de methodiek zoals voorgeschreven voor de Europese Kaderrichtlijn Water. Voor bodem is direct aangesloten op de *technical guidance* documenten (TGD) voor EU risicobeoordelingen van nieuwe en bestaande stoffen en biociden. De overige milieurisicogrenzen, bijvoorbeeld het VR en het ER, zijn onderdeel van het Nederlandse milieubeleid en voor de afleiding van deze risicogrenzen worden aparte procedures beschreven.

Trefwoorden: milieurisicogrenzen, Kaderrichtlijn Water, handleiding, richtsnoer, milieukwaliteitsnormen

Abstract

Guidance for the derivation of environmental risk limits within the framework of 'International and national environmental quality standards for substances in the Netherlands' (INS) - Revision 2007

This report forms the guidance document for the derivation of environmental risk limits used in environmental policy in the Netherlands. The report is a revision of the INS-guidance from 2001. The following four environmental risk limits are distinguished in the Netherlands: negligible concentration (NC), maximum permissible concentration (MPC), serious risk concentration (SRC) and the maximum acceptable concentration for ecosystems (MAC_{eco}).

The guidance document answers the question on what data are needed for the derivation of an environmental risk limit by overviewing and describing how data from the literature should be evaluated for reliability and usefulness. The method of derivation, including the necessary calculations, is described. For water and sediment, the methodology is the same as that prescribed to meet requirements in the European Water Framework Directive. For soil, the methodology for the European risk assessment for new and existing substances and biocides is followed. The remaining risk limits (e.g. NC and SRC) which are required to comply with Dutch environmental policy, are subject to separate derivation procedures. These too are presented here.

Key words: environmental risk limits, Water Framework Directive, guidance, environmental quality standards

Contents

Samenvatting

Dit rapport is de handleiding voor de afleiding van milieurisicogrenzen op het nationale niveau. Dit rapport vervangt de INS handleiding van Traas (2001). Nieuwe elementen in deze handleiding zijn de integratie van de KRW en TGD methodieken en de afleiding van MTRs voor blootstelling van de mens via het milieu.

De afleiding van milieurisicogrenzen vindt plaats binnen het proces '(Inter)nationale Normen Stoffen' (INS), ten behoeve van de uitvoering van het milieubeleid. In Nederland worden de volgende milieurisicogrenzen onderscheiden: het verwaarloosbaar risiconiveau (VR), het maximaal toelaatbaar risiconiveau (MTR), het ernstig risiconiveau (ER) en de maximaal toelaatbare concentratie voor ecosystemen (MAC_{eco}).

De methodiek voor het afleiden van het MTR en de MAC_{eco} voor de milieucompartimenten zoet en zout water en het MTR voor zoetwater-sediment en marien sediment, is gelijk aan de methodiek die onderdeel vormt van de Europese kaderrichtlijn water (KRW). Deze methodiek is vastgelegd in Lepper (2005), die in dit rapport is geïmplementeerd. Volgens de KRW methodiek wordt voor het compartiment water ook een MTR afgeleid die de mens beschermt tegen schadelijke effecten. De methodiek voor MTR afleiding voor het compartiment bodem is gebaseerd op het '*technical guidance document*' (TGD; European Commission, 2003). zoals gebruikt in de Europese risicobeoordeling van nieuwe en bestaande stoffen en biociden. De methodiek voor de afleiding van de overige milieurisicogrenzen is gebaseerd op specifieke Nederlandse procedures. Ook deze procedures worden in dit rapport beschreven. Dit betreft: MTR voor grondwater, VR en ER_{eco} voor alle compartimenten en MTR voor humane blootstelling via bodem, grondwater en lucht.

Om milieurisicogrenzen af te kunnen leiden zijn verscheidene fysische, chemische en toxicologische gegevens nodig. Dit rapport beschrijft gedetailleerd welke parameters nodig zijn en hoe gegevens dienen te worden verzameld, geëvalueerd en geselecteerd voordat met de afleiding van de milieurisicogrenzen wordt begonnen. Daarna volgt een stapsgewijze beschrijving van het afleiden van de risicogrenzen voor de verschillende milieucompartimenten. Daar waar berekeningen plaatsvinden, zijn de benodigde formules gepresenteerd. Een volledige beschrijving van alle parameters en standaardwaarden die in de vergelijkingen worden gebruikt, wordt in het hoofdstuk 'Abbreviations, variables and default values' gegeven. Ook is een korte handleiding opgenomen voor het afleiden van milieurisicogrenzen wanneer die gebaseerd moeten worden op een Europees risicobeoordelingsrapport (EU RAR) voor een bestaande stof.

Summary

This report forms the guidance document for the derivation of environmental risk limits (ERLs) at the Dutch national level. This document replaces the INS guidance by Traas (2001). New elements in this guidance are the integration of WFD guidance, the TGD and the derivation of MPCs for human exposure.

The derivation of environmental risk limits takes place within the process of 'International and national environmental quality standards for substances in the Netherlands' (INS), in order to facilitate environmental policy. The four following ERLs are distinguished in the Netherlands: the negligible concentration (NC), the maximum permissible concentration (MPC), the serious risk concentration (SRC) and the maximum acceptable concentration for ecosystems (MAC_{eco}).

The method for deriving the MPC and MAC_{eco} for freshwater and marine water and the MPC for freshwater and marine sediment, is the same as the guidance, which is part of the European Water Framework Directive (WFD). This methodology is laid down in Lepper (2005), which is implemented in this report. For the water compartment, the ERL derivation according to the WFD methodology includes the derivation of an MPC protecting humans from adverse effects. The methodology for MPC derivation for the soil compartment is based on the technical guidance document (TGD; European Commission, 2003) used for the European risk assessment for new and existing substances, and biocides. The methodology for derivation of the remaining ERLs is based on Dutch procedures. These procedures also are described in this report. These ERLs are: MPC for groundwater; NC, SRC_{eco} for all compartments, and MPCs for human exposure via soil, groundwater and air.

Several physical, chemical and toxicological parameters are needed to derive ERLs. Detailed guidance is given on the parameters needed and how data should be collected, evaluated and selected before the ERL derivation is started. This is followed by a description of the stepwise derivation of the various ERLs for the environmental compartments. The necessary equations are provided where parameters need to be calculated as well as a full description of all parameters and default values used in equations.. Furthermore, guidance is given for ERL derivation in cases where this should be based on the outcomes of a European risk assessment report (EU RAR) for existing substances.

1. Introduction

1.1 Aim and use

The aim of the present report is to provide adequate guidance for the derivation of environmental risk limits (ERLs) used in the Netherlands. The methodology given in the present report should be followed when deriving ERLs. That the methodology is 'guidance' implies that there is room to deviate from the methods described here. Deviating from the guidance is permitted when the circumstances give cause, e.g. when the compound of interest has specific properties or when specific relevant information is available for which guidance has not been developed. Please note that deviating from the guidance should always be motivated in the report describing the ERL derivation and be accompanied by a full description of the alternative method followed.

1.2 Background and sources

This report merges guidance from three different frameworks: the first is the guidance currently used in the Water Framework Directive (WFD, European Commission, 2000), the second is the risk assessment for new and existing substances and biocides (European Commission (Joint Research Centre), 2003a) and the third is ERL derivation specific to the Netherlands (VROM, 2004).

Water Framework Directive
Guidance for the derivation of quality standards in accordance with the European Commission Directive 2000/60/EC (European Commission, 2000) or WFD is laid down in Lepper (2005). This is a revised version of Annex 5 to the report, 'Towards the Derivation of Quality Standards for Priority Substances in the Context of the Water Framework Directive' (Lepper, 2002)[1]. Since Lepper (Lepper, 2005) will be cited regularly in this report, the abbreviation 'FHI' (Fraunhofer Institute) has been used for it. The present report implements FHI guidance in national guidance on ERL derivation for water and sediment, both in the freshwater and marine environment.

New and existing substances and biocides
Guidance for the risk assessment for new and existing substances and biocides is laid down in the 'Technical Guidance Document' or TGD (European Commission (Joint Research Centre), 2003a). In the present report, part II of the TGD will be cited most often; it will be abbreviated by 'TGD'. If other parts than part II of the TGD are cited, a full citation will be given rather than using 'TGD'. In the present report, the TGD is used for ERL derivation for soil.

Please note, however, that the FHI guidance cites the TGD for many topics. Therefore, the TGD is, in fact, present in many other sections of this report as well. It should be noted that although the FHI refers directly to the TGD for the majority of its items, there are also differences between the two documents (Vos and Janssen, 2005). These differences will also be described in detail in this report.

ERL derivation in the Netherlands
Historically, Dutch ERLs are derived within the project INS: 'International and national environmental quality standards for substances in the Netherlands'. The guidance within this project has developed over the years. The most recent guidance document was that by Traas (2001), which

[1] The status of the document prepared by Lepper (2005) is not yet final. DG Environment intends to finalise and publish this document (together with Lepper, 2002) as a 'Manual on the Methodological Framework Used to Derive Quality Standards for Priority Substances of the Water Framework Directive' once the European Commission adopts its proposal (European Commission, 2004b).

became obsolete on 1-1-2004, because the Steering Committee for Substances decided to implement the TGD for derivation of Dutch ERLs. A new national guidance document was not published at that time. Therefore, the report presented here is an updated guidance for the project INS.

In summary, FHI guidance has been followed for water and sediment. For the subjects in this report where the WFD is not applicable, the guidance in this report is in accordance with the TGD. However, for those subjects not covered by the TGD, national guidance is provided. This is part of the process 'International and national environmental quality standards for substances in the Netherlands'.

1.3 Reader's guide

A short overview of the topics dealt with in this guidance is given below.

Chapter 2 describes how data should be (i) collected, (ii) evaluated, (iii) handled (in order to derive useful endpoints), (iv) tabulated and (v) selected for ERL derivation. Detailed information is given on each of these topics.

Chapter 3 describes the methodology for derivation of the MPC. MPC derivation for each of the compartments: water, sediment, soil and groundwater, is described in a separate section. The MPC derivations for human toxicological endpoints for the compartments that are not covered by the FHI guidance (i.e. air, soil and groundwater) are dealt with in a separate section.

Chapter 4 describes how to derive the negligible concentration (NC), the maximum acceptable concentration for ecosystems (MAC_{eco}) and the serious risk concentration for ecosystems (SRC_{eco}). The method for derivation of the SRC_{eco} is revised with respect to its earlier description (Verbruggen *et al.*, 2001) and is now brought in line with TGD guidance.

Chapter 5 describes the methodology to base ERLs on European Union risk assessment reports (EU-RARs).

Chapter 6 explains how species for which ecotoxicological data have been retrieved ('test species') are to be classified taxonomically. The classification presented has been developed within the course of the INS project and has been brought in line with TGD guidance.

A list of references and a list of abbreviations, variables and default values used throughout the report are also given.

Four appendices are added to the report:

Appendix 1 shows so-called 'A1-values' for substances or groups of substances, as listed in EC directive 75/440/EC. These values relate to the quality of surface water intended for drinking-water abstraction. The A1-values are needed in the derivation of MPCs for water.

Appendix 2 shows so-called 'DWS-values' for substances or groups of substances, as listed in EC directive 98/83/EC. These values relate to drinking-water quality ('at the tap') and are needed in the derivation of MPCs for water.

Appendix 3 shows how soils used in ecotoxicological experiments can be classified according to texture. Soil type classification is used when tabulating terrestrial ecotoxicity data.

Appendix 4 gives an overview of terminology and equations associated with partition coefficients.

1.4 Environmental risk limits and environmental quality objectives

Different ERLs, describing four levels of protection, are derived in the Netherlands:

- the negligible concentration (NC) for water, soil, groundwater, sediment and air;
- the maximum permissible concentration (MPC) for water, soil, groundwater, sediment and air, both for ecosystems and for humans;
- the maximum acceptable concentration for ecosystems (MAC_{eco}) for surface water (freshwater and marine);
- the serious risk concentration (SRC) for water, soil, groundwater and sediment, both for ecosystems (SRC_{eco}) and humans (SRC_{human}).

These environmental risk limits (ERLs) serve as advisory values for the setting of environmental quality standards (EQSs). The Dutch Steering Committee for Substances (VROM, 2004) has been appointed to set EQSs. The term EQS is used to designate all legally and non-legally binding standards that are used in Dutch environmental policy.

The term EQS is also used in the FHI document. In the context of the FHI document, EQS is equal to MPC. However, in the Netherlands, the distinction between an ERL and an EQS is very strict (as described above): an MPC can be either a proposed value or a value that is set as an EQS when the Steering Committee for Substances decides to do so. Throughout this document the term MPC is used for the scientifically derived (i.e. proposed) ERL.

1.5 ERLs for ecosystem health and ERLs for human health

An environmental risk limit should represent an *environmental* concentration that protects both humans and ecosystems from adverse effects. For the MPC this is defined as follows (VROM, 1999):
'The MPC has been defined in the policy on substances as the standard based on scientific data which indicates the concentration in an environmental compartment:
1. no effect to be rated as negative is to be expected for ecosystems;
2a no effect to be rated as negative is to be expected for humans (for non-carcinogenic substances);
2b for humans no more than a probability of 10^{-6} per year of death can be calculated (for carcinogenic substances).'[2]

The major part of this report is concerned with the methodology to derive ERLs for ecosystem protection. However, the procedure of deriving ERLs for the protection of human health is also described in this document, always in separate sections, for reasons of clarity.
Figure 1 (page 19) overviews the *final* ERLs that are discerned within the INS framework. Even more ERLs are used in the text of this report. However, all these other ERLs are temporary, e.g. since these ERLs needed to be defined to explain a recalculation method (e.g. wet weight to dry weight, dissolved concentration to total concentration, etc.) or because a selection procedure is applied to come to a final MPC (choice of the final MPC_{water} according to FHI). All MPCs and their descriptions have been listed in the overview of parameters and variables in Table 31.

Two types of ERL are derived for the protection of human health through environmental exposure: the $MPC_{human, comp}$ and the $SRC_{human, comp}$. Both are expressed as a concentration in an environmental compartment, the latter designated by the index 'comp'. These compartments are: soil, water, sediment, groundwater and air and the respective MPCs are called $MPC_{human, soil}$, $MPC_{human, water}$, $MPC_{human, sediment}$, $MPC_{human, gw}$ and $MPC_{human, air}$ These indexes are identical for the $SRC_{human, comp}$. It

[2] This level deviates from the level that has been set in the WFD, where 10^{-6} is defined as a lifetime (70 y) risk (see section 2.4.1). No level has been agreed on in the TGD. In a final draft of a revised chapter for the human health risk characterisation of the TGD, the level of 10^{-6} lifetime risk in deriving limit values for the general population is mentioned in relation to the level used in the EU directives on ambient air and drinking-water quality.

is important to distinguish an *environmental* risk limit (e.g. $MPC_{human, comp}$) from a *human* risk limit (MPC_{human}). The environmental risk limits, like $MPC_{human, comp}$, are compartment concentrations, whereas the human risk limits are intake concentrations. The MPC_{human} is expressed in $\mu g.kg_{bw}^{-1}.d^{-1}$ and is comparable to toxicological threshold values like the TDI (tolerable daily intake).

The SRC values for human health are not derived within the context of the project INS. These values serve as trigger values in the framework of soil remediation in the context of the project 'Risks in Relation to Soil Quality'. The models used to calculate the SRC_{human} values are SEDISOIL and CSOIL (Lijzen *et al.*, 2001).

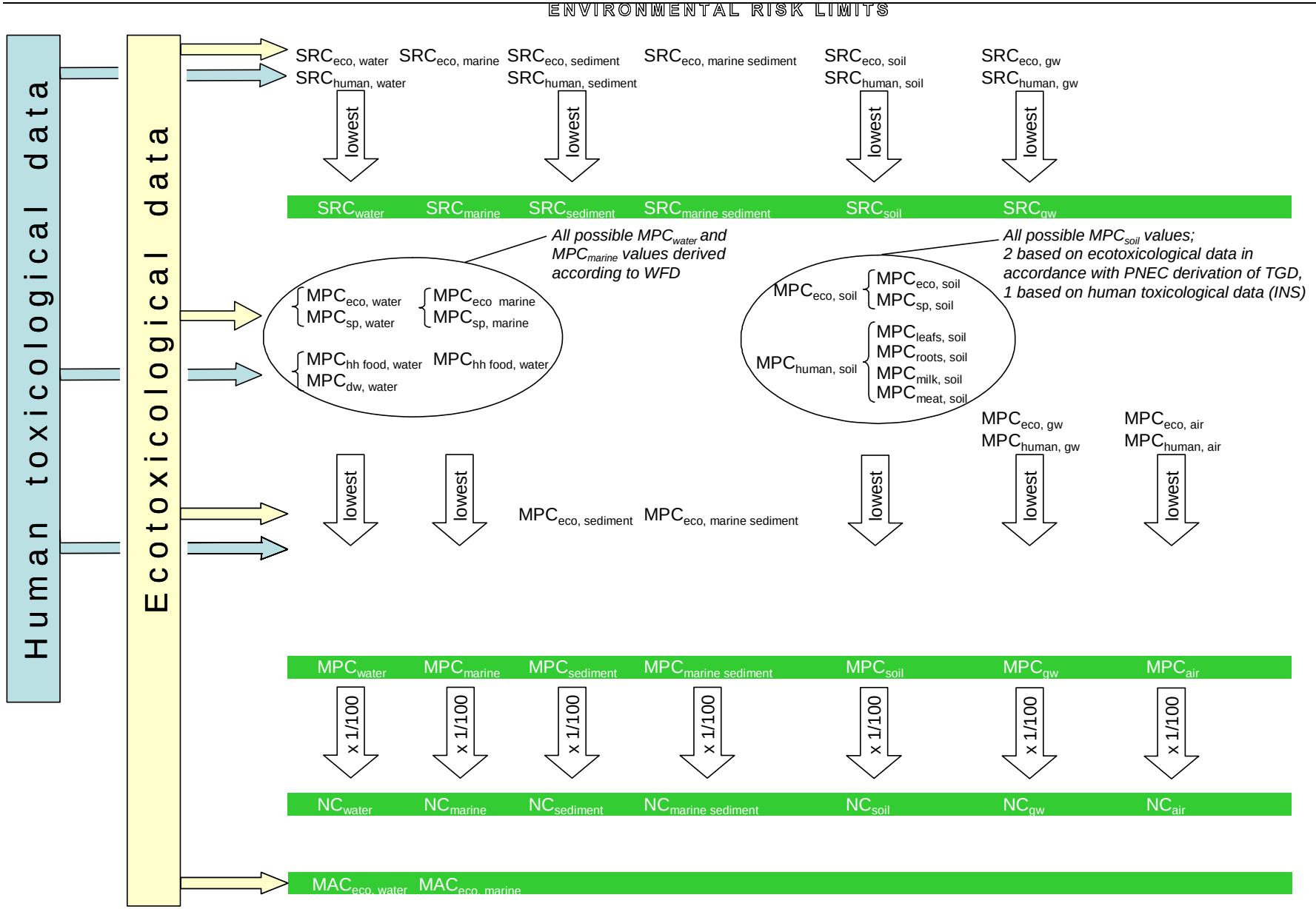

Figure 1. Overview of environmental risk limits within INS framework.
Presented here is a selection scheme. Not indicated are the various possibilities of derivation, e.g. equilibrium partitioning.
Final risk limits are indicated in green. Environmental risk limits protect both humans and ecosystems from exposure to a given compound. The unit of environmental risk limits is: mass of compound per mass (or volume) unit of environmental compartment, expressed as e.g.: $mg.L^{-1}$ or $mg.kg^{-1}$.

Table 1. List of final environmental risk limits discerned within INS framework. Nomenclature and units.

Acronym	Description	Unit[1, 2]
$SRC_{eco, water}$	serious risk concentration for the ecosystem for the freshwater compartment	$mg.L^{-1}$
$SRC_{eco, marine}$	serious risk concentration for the ecosystem for the marine water compartment	$mg.L^{-1}$
$SRC_{eco, sediment}$	serious risk concentration for the ecosystem for the freshwater sediment compartment	$mg.kg_{dw}^{-1}$
$SRC_{eco, marine sediment}$	serious risk concentration for the ecosystem for the marine sediment compartment	$mg.kg_{dw}^{-1}$
$SRC_{eco, soil}$	serious risk concentration for the ecosystem for the soil compartment	$mg.kg_{dw}^{-1}$
$SRC_{eco, gw}$	serious risk concentration for the ecosystem for the groundwater compartment	$mg.L^{-1}$
$SRC_{eco, air}$	serious risk concentration for the ecosystem for the air compartment	$mg.L^{-1}$
$SRC_{human, water}$	serious risk concentration for human health for the freshwater compartment	$mg.L^{-1}$
$SRC_{human, sediment}$	serious risk concentration for human health for the freshwater sediment compartment	$mg.kg_{dw}^{-1}$
$SRC_{human, soil}$	serious risk concentration for human health for the soil compartment	$mg.kg_{dw}^{-1}$
$SRC_{human, gw}$	serious risk concentration for human health for the groundwater compartment	$mg.L^{-1}$
$SRC_{human, air}$	serious risk concentration for human health for the air compartment	$mg.L^{-1}$
SRC_{water}	serious risk concentration for the freshwater compartment	mg.L-1
SRC_{marine}	serious risk concentration for the marine water compartment	$mg.L^{-1}$
$SRC_{sediment}$	serious risk concentration for the freshwater sediment compartment	$mg.kg_{dw}^{-1}$
$SRC_{marine sediment}$	serious risk concentration for the marine sediment compartment	$mg.kg_{dw}^{-1}$
SRC_{soil}	serious risk concentration for the soil compartment	$mg.kg_{dw}^{-1}$
SRC_{gw}	serious risk concentration for the groundwater compartment	$mg.L^{-1}$
SRC_{air}	serious risk concentration for the air compartment	$mg.L^{-1}$
MAC_{eco}	maximum acceptable concentration for the ecosystem for the water compartment	$mg.L^{-1}$
$MPC_{eco, water}$	maximum permissible concentration for the ecosystem for the freshwater compartment	$mg.L^{-1}$
$MPC_{eco, marine}$	maximum permissible concentration for the ecosystem for the marine water compartment	$mg.L^{-1}$
$MPC_{eco, sediment}$	maximum permissible concentration for the ecosystem for the freshwater sediment compartment	$mg.kg_{dw}^{-1}$
$MPC_{eco, marine sediment}$	maximum permissible concentration for the ecosystem for the marine sediment compartment	$mg.kg_{dw}^{-1}$
$MPC_{eco, soil}$	maximum permissible concentration for the ecosystem for the soil compartment	$mg.kg_{dw}^{-1}$
$MPC_{eco, gw}$	maximum permissible concentration for the ecosystem for the groundwater compartment	$mg.L^{-1}$
$MPC_{eco, air}$	maximum permissible concentration for the ecosystem for the air compartment	$mg.L^{-1}$
$MPC_{dw, water}$	maximum permissible concentration for drinking-water abstraction for the freshwater compartment	
$MPC_{hh food, water}$	maximum permissible concentration for human consumption of fishery products for the freshwater and marine water compartment	$mg.L^{-1}$
$MPC_{sp, marine}$	maximum permissible concentration for secondary poisoning for the marine water compartment	$mg.L^{-1}$
$MPC_{sp, soil}$	maximum permissible concentration for secondary poisoning for the for the soil compartment	$mg.kg_{dw}^{-1}$
$MPC_{sp, water}$	maximum permissible concentration for secondary poisoning for the freshwater compartment	$mg.L^{-1}$
$MPC_{human, water}$	maximum permissible concentration for human health for the freshwater compartment	$mg.L^{-1}$
$MPC_{human, soil}$	maximum permissible concentration for human health for the soil compartment	$mg.kg_{dw}^{-1}$
$MPC_{human, gw}$	maximum permissible concentration for human health for the groundwater compartment	$mg.L^{-1}$
$MPC_{human, air}$	maximum permissible concentration for human health for the air compartment	$mg.L^{-1}$
MPC_{water}	maximum permissible concentration for the freshwater compartment	$mg.L^{-1}$
MPC_{marine}	maximum permissible concentration for the marine water compartment	$mg.L^{-1}$
$MPC_{sediment}$	maximum permissible concentration for the freshwater sediment compartment	$mg.kg_{dw}^{-1}$
$MPC_{marine sediment}$	maximum permissible concentration for the marine sediment compartment	$mg.kg_{dw}^{-1}$
MPC_{soil}	maximum permissible concentration for the soil compartment	$mg.kg_{dw}^{-1}$
MPC_{gw}	maximum permissible concentration for the groundwater compartment	$mg.L^{-1}$
MPC_{air}	maximum permissible concentration for the air compartment	$mg.L^{-1}$
NC_{water}	negligible concentration for the freshwater compartment	$mg.L^{-1}$
NC_{marine}	negligible concentration for the marine water compartment	$mg.L^{-1}$

Acronym	Description	Unit[1, 2]
$NC_{sediment}$	negligible concentration for the freshwater sediment compartment	$mg.kg_{dw}^{-1}$
$NC_{marine\ sediment}$	negligible concentration for the marine sediment compartment	$mg.kg_{dw}^{-1}$
NC_{soil}	negligible concentration for the soil compartment	$mg.kg_{dw}^{-1}$
NC_{gw}	negligible concentration for the groundwater compartment	$mg.L^{-1}$
NC_{air}	negligible concentration for the air compartment	$mg.L^{-1}$

[1] The unit 'mg' is optional (e.g. µg might also be used, if convenient).
[2] ERLs for sediment and soil are expressed per kg dry weight of Dutch standard sediment and kg dry weight of Dutch standard soil, respectively.

1.6 Standard soil, sediment and suspended matter

The methodology for derivation of ERLs for soil and sediment in this report, makes use of the characteristics for Dutch standard soil, Dutch standard sediment and Dutch standard suspended matter as they have been used in the past for ERL derivations at the Dutch national level. These characteristics are: the percentage of organic matter, which is proportional to the percentage organic carbon, the percentage of clay (lutum), and the concentration of suspended matter in surface water. The ERLs should be expressed on the basis of Dutch characteristics.

Note that an ERL that is expressed in standard soil or sediment should be recalculated to local soil or sediment conditions when a local concentration is compared with an ERL (VROM, 1999). Using Dutch standard conditions for all ERLs is thus a way of expressing ERLs, a systematisation that enables comparison of values for different compounds, rather than a generic value that should be valid for all soils and sediments in the Netherlands.

In the FHI and TGD guidance documents, these characteristics have values that differ from the standards used in the Netherlands. FHI follows the TGD for the percentages of organic matter or organic carbon in sediment and suspended matter (Table 2).

Table 2. Characteristics of standard soil, standard sediment and standard suspended matter used in INS compared to TGD and FHI guidance.

	INS (Netherlands)				TGD and FHI		
Parameter / Compartment	% o.m. [-]	% o.c. [-]	% clay [-]	C_{susp} [$mg.L^{-1}$l]	% o.m. [-]	% o.c. [-]	C_{susp} [$mg.L^{-1}$]
soil	10	5.88	25	–	3.4	2	–
suspended matter	20	11.8	40	30	17	10	15
sediment	10	5.88	25	–	8.5	5	–

Values based on VROM (VROM, 1999), EC (2003a) and Lepper (2005).

2. Data collection and evaluation

Before any data are collected, a check should be performed to see if there are EU-RAR documents available for the compounds of interest (Regulation (EC) No. 793/93) or whether the compound is on the list of priority substances of the Water Framework Directive. It is recommended to use the ESIS (European chemical Substances Information System) database on the internet (http://ecb.jrc.it/esis/) to trace any EU-RAR documents.

- For compounds for which an EU-RAR is in draft, no risk limits will be derived (in compliance with the current policy of the Ministry of VROM).
- For compounds for which a finalised EU-RAR is available, the PNECs are recalculated to MPCs (see Chapter 5), making use of the Dutch characteristics for soil, sediment and suspended matter (see section 1.6). The following PNECs are used: $PNEC_{water}$, $PNEC_{marine}$, $PNEC_{sediment}$, $PNEC_{marine\ sediment}$, and $PNEC_{soil}$. The data validated in the EU-RAR should be used to derive the SRC_{eco} and if applicable, the MAC_{eco}. PNECs for these compartments are not given in the section on risk assessment for human health in an EU-RAR. From the risk assessment and the EUSES calculation presented, MPC values should be derived for human health as well (see sections 3.1.5 and 3.1.6 for water and 3.3.6 for other compartments).
- For compounds that are priority substances in the Water Framework Directive, annual average quality standards (AA-QS) values for freshwater, marine water, freshwater sediment and marine sediment are available in principle, plus a MAC-QS for freshwater. For the Dutch situation, the AA-QS-values are taken over as MPC and the MAC-QS as MAC_{eco}. The data validated in the WFD fact sheets should be used to derive the SRC_{eco}., ERLs are also derived for other compartments (soil, groundwater and air, if applicable) in the framework of INS. Additional literature searches should be performed for these compartments.

The toxicity data that are used to derive the environmental risk limits for plant protection products (PPP) comprise both all publicly available literature data and all confidential data. The confidential data for plant protection products should be made available by the Dutch Board for Authorisation of Pesticides (CTB). If more than one registration dossier for the same compound (active substance) is available, data from all registration dossiers should be taken into account when deriving environmental risk limits. According to the FHI-guidance, the data[3] validated in the risk assessments under Directives 98/8/EC (biocides) or 91/414/EEC (plant protection products) should be used for EQS-setting with the highest priority, to assure coherence with other EU legislation. Any relevant information provided by companies can also be evaluated for use in the ERL derivation.

2.1 Physicochemical data

2.1.1 Data collection

2.1.1.1 Identity

The following data on substance identity are collected:

- IUPAC name
- structural formula
- CAS registry number
- EINECS number

[3] Only validated data will be used, not the risk assessments. These data were already subject to extensive review and can be used without any additional evaluation.

- chemical formula[4]
- SMILES code

IUPAC name, CAS registry number, EINECS number and empirical formula are primarily derived from the ESIS database (ECB website, http://ecb.jrc.it/esis/). A structural formula can also be obtained here for a great number of compounds. If a structural formula can not be obtained from the ESIS database, EPI Suite software can be used (U.S. EPA, 2007b), or handbooks can be consulted, e.g. Tomlin (2002) for pesticides or more general handbooks like Mackay *et al*. (2006). The SMILES code is generated by EPI Suite software. If the compound of interest is not available in the EPI Suite database, the SMILES code can be generated using e.g. the ChemSketch (ACD/Labs, 2006) software.

2.1.1.2 Physicochemical properties

Physicochemical parameters should be collected for each compound for which ERLs are derived. These parameters provide information on the behaviour of the compound in the environment. Data on the following parameters are collected (name, symbol, unit):

- molecular weight: M_w, (g.mol^{-1});
- melting point: T_m, (°C);
- boiling point: T_b, (°C);
- vapour pressure: P_v (Pa), experimental melting point and boiling point can be useful for estimation of the vapour pressure;
- Henry's law constant: H (Pa.m^3.mol^{-1}).
- water solubility: S_w (mg.L^{-1}), experimental melting point can be useful for the estimation of the solubility from log K_{ow};
- dissociation constant: pK_a (-);
- *n*-Octanol/water partition coefficient: K_{ow} (-);
- soil/sediment water partition coefficient: K_p, (L.kg^{-1}). For organic substances, the partition coefficients normalised to organic carbon are preferred: K_{oc} (L.kg^{-1}). For metals, field based partition coefficients (K_p) are searched for, both for soil and suspended matter;

The following steps should preferably be followed to collect physicochemical data:

1. The following databases and estimation methods are used to retrieve or calculate data on physicochemical parameters (Table 3).

Table 3. Sources and estimation methods to be screened for physicochemical parameters.

Parameter	**Sources/methods**
M_W	**Mackay, EPI Suite, SPARC, IUCLID**
T_m	**Mackay, EPI Suite, IUCLID**
T_b	**Mackay, EPI Suite, SPARC, IUCLID**
P_v	**Mackay, EPI Suite, SPARC, IUCLID**
H	**Mackay, BioLoom, EPI Suite, SPARC, IUCLID**
S_w	**Mackay, EPI Suite, SPARC, IUCLID**
pK_a	**Mackay, BioLoom, SPARC, IUCLID**
K_{ow}	**BioLoom, Mackay, EPI Suite, SPARC, IUCLID**
K_{oc}	**Mackay, BioLoom, Sabljić, EPI Suite, IUCLID**
K_p (metals)	**Sauvé, Bockting, scientific literature**

References to the sources and programs mentioned in Table 3:

Mackay = Mackay *et al*. (2006);
EPI Suite = U.S. EPA (2007b);
SPARC = SPARC online calculator (2007);

[4] In Dutch: bruto formula.

IUCLID = International Uniform Chemical Information Database (European Commission (European Chemical Bureau), 2000);
Bioloom = BioByte including internet database (BioByte, 2004);
Sabljić = Sabljić and Güsten (1995) cited in: European Commission (2003b) or Sabljić *et al*. (1995).
Sauvé = Sauvé *et al*., (2000)
Bockting = Bockting *et al*., (1992)

2. Scientific literature. For all of the listed parameters, the open literature may, in principle, be searched (method, see section 2.2.1) in the case that a reliable estimate is lacking or if the number of reliable or relevant data is very low. This might be most applicable to K_p values for metals (see section 2.1.2.6) since a robust data collection in this area is absent.
3. Contact persons from environmental agencies in other countries are consulted by sending out an e-mail enquiry, in which they are asked if they have access to specific information on ecotoxicological toxicity data (see section 2.2.1) and/or physicochemical data and are willing to share those data.
4. The industry parties involved in production or use of the compounds under investigation are invited to submit relevant studies, which will be treated as public literature.

2.1.2 Data evaluation and data tables

All retrieved literature is read and evaluated with respect to its usefulness and reliability. Several aspects considered important for the evaluation of the parameters, are discussed in the following sections.

After evaluating a study, the results of the study are summarised by entering these into the appropriate data table (Table 4). The structural formula of the compound is also placed in this table.

Table 4. Overview and default table structure for identity- and physicochemical parameters listed for each compound.

Properties	Value	Reference
IUPAC Name		
Structural formula		
CAS number		
EINECS number		
Chemical formula		
SMILES code		
Molecular weight ($g.mol^{-1}$)		
Melting point (°C)		
Boiling point (°C)		
Vapour pressure (Pa)		
Henry's law constant ($Pa.m^3.mol^{-1}$)		
Water solubility ($mg.L^{-1}$)		
pK_a		
n-Octanol/water partition coefficient (log K_{ow})		
Soil or sediment/water sorption coefficient (log K_{oc})		
Soil or sediment/water sorption coefficient (log K_p)		
Suspended matter/water partition coefficient		

2.1.2.1 Evaluation of the vapour pressure for use in ERL derivation

An OECD guideline exists for the experimental determination of the vapour pressure of a compound (OECD guideline 104; OECD, 1995b). In this guideline several methods are discussed, each with its own range of applicability. The following table presents information from the guideline, which specifies what method is suitable for which compound.

Table 5: Domain of applicability of different methods for the determination of vapour pressure.

Method	Suitable for liquids	Suitable for solids	Recommended range
Dynamic method	low melting	yes	10^3-10^5 Pa
Static method	Yes	yes	10-10^5 Pa
Isoteniscope	Yes	yes	10^2-10^5 Pa
Effusion method	Yes	yes	10^{-3}-1 Pa
Gas saturation method	Yes	yes	10^{-5}-10^3 Pa
Spinning rotor method	Yes	yes	10^{-4}-0.5 Pa

In the dynamic method (Cottrell's method), the boiling point of a compound is determined at various pressures between about 10^3 and 10^5 Pa. In the static method, the vapour pressure is determined at one specified temperature by means of a manometer (e.g. 25 ºC). The isoteniscope method is based on the same principle as the static method. In the effusion method the weight loss of the compound is measured. This can be done directly by measuring the mass of the remaining substance or by analysing the volatilised amount by gas chromatography (GC). In the proposed update of guideline 104 (OECD, 2002), isothermal gravimetry is added for the effusion method. The weight loss is then determined at different temperatures and an extrapolation to 20 or 25 ºC can be made. The range of vapour pressures that can be determined with this method is 10^{-10} to 1 Pa. The gas saturation method makes use of a column containing a carrier material supporting the substance, through which an inert gas is passed. The concentration of the substance in this carrier gas is then determined, usually by gas chromatography (GC). The last method is the spinning rotor method, where the retardation of a spinning ball due to the friction with the gas phase is measured.

In general, the methods that make use of an analysis of the substance, for example, by gas chromatography, are less prone to errors due to impurities than the other methods. The OECD guideline does not mention this explicitly. However, degassing of more volatile compounds prior to the determination of the vapour pressure also enhances the reliability of the determination.

The retention time in gas chromatography can be used to estimate the vapour pressure of a compound. Although this is not a direct determination of the vapour pressure, it generally gives rather accurate results and is applicable to substances with a very low vapour pressure. In addition to this, the vapour pressure can be estimated by the programme MPBPwin, which is incorporated in EPI Suite (U.S. EPA, 2007b). The programme makes use of three estimation methods, which are the Antoine method, the modified Grain method and the Mackay method. All three methods make use of the boiling point for their estimation of the vapour pressure. Also the melting point of the compound is a necessary parameter for the estimation. Both boiling and melting point can be estimated by the programme, but experimental values can also be entered if known. For solids, the result of the modified Grain method is presented as the preferred value, while for liquids this is the mean of the Antoine method and the modified Grain method. A value for the vapour pressure can also be estimated by SPARC (Karickhoff *et al.*, 2007), which has a mechanistic thermodynamic basis. In the data tables, both estimated values are reported as well.

2.1.2.2 Henry coefficient

No general accepted guideline exists for the determination of the Henry coefficient. However, several methods exist to determine the Henry coefficient experimentally.

In the batch stripping method, gas is bubbled at a known rate through a solution of the compound in water. The Henry coefficient is calculated with a mass balance from the decrease in the aqueous concentration. The concentration in air is generally not measured. This method works well for fairly volatile compounds with Henry coefficients higher than 2.5 and occasionally down to 0.25 $Pa.m^3.mol^{-1}$ (Mackay *et al.*, 2000).

One common method, very similar to the batch stripping method, is the gas stripping method in which a gas is bubbled through the aqueous solution and both the aqueous concentration and the gas concentration are determined. The technique was applied to chlorobenzenes, PAHs, and PCBs in a range from 0.018 to 276 $Pa.m^3.mol^{-1}$ (Ten Hulscher *et al.*, 1992).

A method for highly volatile compounds (i.e. higher than 120 $Pa.m^3.mol^{-1}$) is the Equilibrium Partitioning In Closed Systems (EPICS) method. With this method a known volume of solute in water solution is equilibrated with air in sealed vessels. The headspace air concentrations are measured. The method has a high precision (Mackay *et al.*, 2000). A number of other headspace analysis techniques that are used, are slightly different from the EPICS method, in some techniques not only the headspace but both phases are analysed (Mackay *et al.*, 2000).

A method for less volatile compounds is the wetted-wall method. In this method the solute is equilibrated between a thin flowing film of water and a concurrent air flow in a vertical column. Both phases are measured. The method has been applied to pesticides and other less volatile compounds, but no recommended range is given (Mackay *et al.*, 2000). In the handbook (Mackay *et al.*, 2006), values for polychlorinated biphenyls (PCBs), polyaromatic hydrocarbons (PAHs), and two pesticides are tabulated using this method. Values for PCBs and PAHs range from 0.91 to 74.3 $Pa.m^3.mol^{-1}$. One of the pesticides (alachlor) has a much lower Henry coefficient of $8.43 \cdot 10^{-4}$ $Pa.m^3.mol^{-1}$. This is in agreement with the method being suitable for less volatile compounds.

Also the Henry coefficient is sometimes related to retention times (Mackay *et al.*, 2000). However, results obtained using this method should be considered as an estimate. Another estimation that is often used for the Henry coefficient is the quotient of vapour pressure and solubility. This method works quite well for substances that have a solubility of less than 1% in water. The Henry coefficient can also be calculated by a bond contribution method as included in EPI Suite (U.S. EPA, 2007b). These estimated values should be included in the data table.

2.1.2.3 Evaluation of the water solubility for use in ERL derivation

For the experimental determination of the water solubility, an OECD guideline is available (OECD guideline 105; OECD, 1995c), in which two methods are discussed. These methods are the flask method (shake-flask) and the column elution method (generator column). The flask method can be used for compounds with a solubility higher than 10 $mg.L^{-1}$. Below that value, colloid formation will overestimate the true aqueous solubility and in that case the column elution method should be used, which prevents this phenomenon.

Apart from the methods proposed in the OECD guideline, the water solubility of poorly soluble liquid compounds can be accurately determined by means of the slow-stirring method. The reliability of the slow-stirring method applied to liquid substances can be considered as equivalent to that of the column elution method. Only few examples are available of the use of this method for the determination of the solubility, mostly for hydrocarbons and phthalate esters (Tolls *et al.*, 2002; Letinski *et al.*, 2002; Ellington, 1999). This method is often used to prepare saturated solutions of hydrocarbon mixtures (oil products) in water (water accommodated fractions or WAF), by which information on the solubility of a mixture is given (Schluep *et al.*, 2002).

Estimates of the water solubility can be made by two different programmes included in EPI Suite (U.S. EPA, 2007b). These programmes are WSKOWwin, which estimates the solubility from log K_{ow}, and WATERnt, which is a fragment method for water solubility independent of log K_{ow}. Experimental values for log K_{ow} and melting point can be entered in WSKOWwin if available.

Otherwise WSKOWwin will use the default values (experimental or calculated) from EPI Suite for these parameters. Another estimation method for the water solubility is the calculation performed by SPARC (Karickhoff *et al.*, 2007), which has a mechanistic thermodynamic basis. These estimated values are reported as well in the data tables.

2.1.2.4 Evaluation of K_{ow} values for use in ERL derivation

Several methods are available for the experimental determination of log K_{ow}. In the OECD guidelines, two methods are available and further there is one draft guideline. The first method is the shake-flask method (OECD guideline 107; OECD, 1995a). This method works well for log K_{ow} values in the range between -2 and 4 (occasionally up to 5), but is impossible to use with surface-active materials. For these materials, a calculated value (using BioLoom; BioByte, 2004) or an estimate based on individual *n*-octanol solubility and water solubility should be provided, preferably in mutually saturated *n*-octanol and water (Sijm *et al.*, 1999; Li and Yalkowsky, 1998a; Li and Yalkowsky, 1998b).

The second method is the HPLC method. Values of log K_{ow} in the range between 0 and 6 can be estimated using high performance liquid chromatography (OECD guideline 117; OECD, 2004). The HPLC method is not applicable to strong acids and bases, metal complexes, surface-active materials or substances which react with the eluent. The HPLC method is less sensitive to the presence of impurities in the test compound than is the shake-flask method. Nevertheless, in some cases impurities can make the interpretation of the results difficult because peak assignment becomes uncertain. For mixtures which give an unresolved band, upper and lower limits of log K_{ow} should be stated.

Before deciding on what procedure to use, a preliminary estimate of the log K_{ow} should be obtained from calculation (see the annex to Guideline 117), or where appropriate from the ratio of the solubilities of the test substance in the pure solvents. Still, the HPLC method should be regarded as an estimation method of the log K_{ow}, because it does not directly measure the distribution of a compound between octanol and water.

Another method that determines the distribution of a compound between *n*-octanol and water directly, but whose reach extends beyond the range of the shake-flask method, is the slow-stirring method (draft OECD guideline 123; OECD, 2003). With this method, log K_{ow} values up to 8.2 can be accurately determined, making it suitable for highly hydrophobic compounds. This method prevents the formation of micro droplets of *n*-octanol in the aqueous phase, which results in an overestimation of the water concentration and, consequently, an underestimation of the log K_{ow} value. For the same reason, the shake-flask method can only be used up to log K_{ow} values of around 4 and definitely not higher than 5.

Another method that is not mentioned in OECD guidelines is the generator-column technique. Although this technique is most frequently used for the determination of the water solubility, it is occasionally used for the determination of log K_{ow}. Because the supporting material silica, saturated with *n*-octanol containing the compound, is held in a column, the formation of micro droplets is excluded. For this reason, the results from this technique can be considered equivalent to results obtained with the slow-stirring method. In general, good correlation exists between the slow-stirring method and the generator-column technique, within the experimental error of both methods. However, only a limited number of studies is available that makes use of this technique, primarily for chlorinated biphenyls and dibenzodioxins (e.g. Tewari *et al.*, 1982; Miller *et al.*, 1984; Doucette and Andren, 1987; Doucette and Andren, 1988; Hawker and Connell, 1988; Shiu *et al.*, 1988; Li and Doucette, 1993; Yeh and Hong, 2002).

Except from experimental determination, log K_{ow} values can also be calculated with a QSAR programme. The log K_{ow} values calculated with ClogP (BioByte, 2004) and EPI Suite (U.S. EPA, 2007b) are always presented for comparison. Both programmes are based on a fragment contribution method. Besides this, SPARC (Karickhoff *et al.*, 2007) is a third estimation programme for the log K_{ow} that is frequently used. This programme is not based on a fragment contribution but has a mechanistic thermodynamic basis.

2.1.2.5 Evaluation of K_{oc} values for use in ERL derivation

The organic carbon normalised partition coefficient (K_{oc}) is calculated or directly retrieved from literature for all valid adsorption studies collected. The soil or sediment type that underlies these partition coefficients is reported (e.g. sediment, loamy sand, suspended matter) in the table. The organic carbon content is also reported. The method to determine the K_{oc} most accurately is the OECD guideline 106 (OECD, 2000). All K_{oc} values that are determined with a method similar to this guideline can be regarded as reliable. However, the TGD also allows K_{oc} values to be derived from field studies or simulation studies. Therefore, whether or not a sorption study is reliable remains subject to expert judgement.

The K_{oc} may also be calculated. Estimation of K_{oc} from K_{ow} is the preferred route, following the QSAR method described in the TGD (cited in the next section). A short description of the use of the method is given after the citation.

Citation from TGD, part III (European Commission (Joint Research Centre), 2003b):

> 'The models are based on linear regression analysis and log K_{ow} as descriptor variable. It should be noted that all models are developed assuming an equilibrium state. For certain classes of chemicals, e.g. anilines and carbamates, this assumption is not correct, because the sorption to soil is irreversible due to the formation of bonded residues. Improvements of the more specific models is certainly feasible if parameters for more specific interactions are taking into account.'
>
> '*Domain*
> An extensive description of the domain is given in Table 6[5]. The description is made in terms of chemical structures as well as in terms of log K_{ow} ranges.
>
> *Accuracy*
> The standard errors of the estimates (± 2σ range = 95%)[6] range from 0.35 to 1.0 log units for the different models. The standard errors are indicated in Table 7[5] for each model. A cross-validation has not been performed yet. External validation is not possible, because all available data have been used to generate the models (Sabljić *et al.*, 1995 cited in: European Commission (Joint Research Centre), 2003a).'

[5] The number of the table refers to this document and not the table number in the TGD.
[6] For clarification, the standard error is equal to σ.

Table 6. Domain of the sorption models (Sabljić et al., 1995 cited in: European Commission (Joint Research Centre), 2003a).

Model	X-variable domain log K_{ow} in log units	Chemical domain	Substituents or Warnings
Hydrophobics	1 - 7.5	All chemicals with C, H, F, Cl, Br, and I atoms	
Nonhydrophobics	(-2.0) - 8.0	All chemicals that are not classified as hydrophobics	Overestimated *n*-Alkyl Alcohols (0.9 log units) Organic Acids (0.55 log units) Underestimated Amino-PAHs (1-2 log units) Aliphatic Amines (1-2 log units) Alkyl Ureas (1.0-1.5 log units)
Phenols	1.0 - 5.0	Phenols	Cl, Br, CH_3, OH, NO_2, CH_3O
		Anilines	Cl, Br, CH_3, CF_3, CH_3O, N-Me
		Benzonitriles	Chlorinated
		Nitrobenzenes	Cl, Br, NH_2
Agricultural	(-1.0) - 8.0	Acetanilides	
		Carbamates	
		Esters	
		Phenylureas	
		Phosphates	
		Triazines	
		Uracils	
Alcohols, acids	(-1.0) - 5.0	Alcohols	Alkyl, Phenalkyl, OH
		Organic Acids	All
Acetanilides	0.9 - 5.0	Anilides	CH_3O, Cl, Br, NO_2, CF_3, CH_3
Alcohols	(-1.0) - 5.0	Alcohols	Alkyl, Phenalkyl, OH
Amides	(-1.0) - 4.0	Acetamides	F, Cl, Br, CH_3O, Alkyl
		Benzamides	NO_2, N-Me
Anilines	1.0 - 5.1	Anilines	Cl, Br, CF_3, CH_3, N-Me, N, N-di-Me
Carbamates	(-1.0) - 5.0	Carbamates	Alkyl, Alkenyl, Cl, Br, N-Me, CH_3O
Dinitroanilines	0.5 - 5.5	Dinitroanilines	CF_3, Alkyl-SO_2, NH_2SO_2, CH_3, *t*-Bu
Esters	1.0- 8.0	Phthalates	alkyl, phenyl, Cl
		Benzoates	alkyl, phenyl, NO_2,OH,Cl,NH_2
		Phenylacetates	alkyl, phenalkyl
		Hexanoates	alkyl
		Heptanoates	alkyl
		Octanoates	alkyl
Nitrobenzenes	1.0 - 4.5	Nitrobenzenes	Cl, Br, NH_2
Organic Acids	(-0.5) - 4.0	Organic Acids	All
Phenols	0.5 - 5.5	Phenols	Cl, Br, NO_2, CH_3, CH_3O, OH
		Benzonitriles	Cl
Phenylureas	0.5 - 4.2	Phenylureas	CH_3, CH_3O, F, Cl, Br, Cyclo-alkyls, CF_3, PhO
Phosphates	0.0 - 6.5	All Phosphates	
Triazines	1.5 - 4.0	Triazines	Cl, CH_3O, CH_3S, NH_2, N-Alkyl
Triazoles	(-1.0) - 5.0	Triazoles	Alkyl, CH_3O, F, Cl, CF_3, NH_2

Table 7. QSARs for soil and sediment sorption for different chemical classes (Sabljić et al., 1995 cited in European Commission (Joint Research Centre), 2003a).

Chemical class	Equation	Statistics
Predominantly hydrophobics	$\log K_{oc} = 0.81 \log K_{ow} + 0.10$	n=81, r^2=0.89, s.e.=0.45
Nonhydrophobics	$\log K_{oc} = 0.52 \log K_{ow} + 1.02$	n=390, r^2=0.63, s.e.=0.56
Phenols, anilines, benzonitriles, nitrobenzenes	$\log K_{oc} = 0.63 \log K_{ow} + 0.90$	n=54, r^2=0.75, s.e.=0.40
Acetanilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, uracils	$\log K_{oc} = 0.47 \log K_{ow} + 1.09$	n=216, r^2=0.68, s.e.=0.43
Alcohols, organic acids	$\log K_{oc} = 0.47 \log K_{ow} + 0.50$	n=36, r^2=0.72, s.e.=0.39
Acetanilides	$\log K_{oc} = 0.40 \log K_{ow} + 1.12$	n=21, r^2=0.51, s.e.=0.34
Alcohols	$\log K_{oc} = 0.39 \log K_{ow} + 0.50$	n=13, r^2=0.77, s.e.=0.40
Amides	$\log K_{oc} = 0.33 \log K_{ow} + 1.25$	n=28, r^2=0.46, s.e.=0.49
Anilines	$\log K_{oc} = 0.62 \log K_{ow} + 0.85$	n=20, r^2=0.82, s.e.=0.34
Carbamates	$\log K_{oc} = 0.37 \log K_{ow} + 1.14$	n=43, r^2=0.58, s.e.=0.41
Dinitroanilines	$\log K_{oc} = 0.38 \log K_{ow} + 1.92$	n=20, r^2=0.83, s.e.=0.24
Esters	$\log K_{oc} = 0.49 \log K_{ow} + 1.05$	n=25, r^2=0.76, s.e.=0.46
Nitrobenzenes	$\log K_{oc} = 0.77 \log K_{ow} + 0.55$	n=10, r^2=0.70, s.e.=0.58
Organic acids	$\log K_{oc} = 0.60 \log K_{ow} + 0.32$	n=23, r^2=0.75, s.e.=0.34
Phenols, benzonitriles	$\log K_{oc} = 0.57 \log K_{ow} + 1.08$	n=24, r^2=0.75, s.e.=0.37
Phenylureas	$\log K_{oc} = 0.49 \log K_{ow} + 1.05$	n=52, r^2=0.62, s.e.=0.34
Phosphates	$\log K_{oc} = 0.49 \log K_{ow} + 1.17$	n=41, r^2=0.73, s.e.=0.45
Triazines	$\log K_{oc} = 0.30 \log K_{ow} + 1.50$	n=16, r^2=0.32, s.e.=0.38
Triazoles	$\log K_{oc} = 0.47 \log K_{ow} + 1.41$	n=15, r^2=0.66, s.e.=0.48

n is the number of data, r^2 is the correlation coefficient and s.e. the standard error of estimate.

End of citation

The QSARs in Table 7 are from a report cited in the TGD, but they can also be found in the public literature (Sabljić *et al*., 1995). In principle, the appropriate QSAR should be chosen on basis of this table. For many compounds with polar groups attached, a separate QSAR is available for that particular chemical class. In general, these QSARs do not deviate very much from the QSARs for larger subsets of chemical classes. However, if there is doubt about which QSAR to use, for example, due to the presence of more than one functional group, it is often most convenient to use the more general QSARs, in particular the QSAR for non-hydrophobic chemicals. This QSAR, together with the QSAR for predominantly hydrophobic compounds provides a reasonable estimate of the K_{oc} for most compounds.

The K_{oc} can also be estimated with an HPLC method (OECD guideline 121; OECD, 2001). As the title of the method indicates, this is no direct determination of the K_{oc} but an estimate based on another property (retention in HPLC). Also the estimation routine PCKOCwin, which employs a calculation method based on molecular connectivity indices (MCI), may be used to estimate the K_{oc}. PCKOCwin is embedded in the EPI Suite software (U.S. EPA, 2007b). Both methods can aid in the decision by means of an independent estimation, in the case that the interpretation of the estimation method based on log K_{ow} according to the TGD is difficult. Both the estimated value from molecular connectivity and values estimated with the HPLC method, if any available, should be reported.

2.1.2.6 Evaluation of K_p values for metals for use in ERL derivation

Adsorption of metals to the solid fraction of soil, sediment or particulate (suspended) matter is dependent on many variables such as cation exchange capacity, organic matter content and clay content, pH, redox potential, etc. In contrast to organic compounds, there is no estimation method to predict metal-solids partitioning in environmental compartments from compound properties. Thus, partition coefficients for metals have to be determined in and retrieved from experimental studies.

The K_p values are collected from all valid studies reporting metal partition coefficients.

Relevant studies are those that report K_p values for sediment, soil or suspended matter (or K_d values) determined in *field* samples. Batch adsorption studies, performed in the laboratory, are a second type of potentially relevant studies. An established data source of metal K_p values for bulk compartments (soil, sediment, suspended matter) does – to our knowledge– not exist. A few references that are of interest are Sauvé *et al*. (2000) and Bockting *et al*. (1992), although values of the latter have been criticised (Koops *et al.*, 1998). Due to the heterogeneity of adsorbents encountered in various compartments, K_p values for metals usually show a high variation. Since normalisation is generally impracticable, selection of the K_p value(s) to be used in EqP needs careful consideration.

2.1.3 Data selection

2.1.3.1 K_{ow}

The K_{ow} value that is selected for use in the ERL derivation is preferably the selected experimental value (MlogP) presented by BioLoom (BioByte, 2004). This value is assigned the highest quality in the underlying database (MedChem). Only if this database does not give a selected value or when careful considerations lead to a different selection, the selected (log) K_{ow} value is the average value of all reliable values determined by the shake flask, slow stirring or generator column method, for which guidance is given in section 2.1.2.4. This selected log K_{ow} is reported as described in section 3.1.1 (Table 15). K_{ow} values estimated using the HPLC method are indirect estimates of octanol/water partitioning and are therefore not regarded as most reliable, they are not used when more reliable data are available.
When no or only unreliable experimental data on K_{ow} are available, the selected data should be calculated with a QSAR programme. The use of the K_{ow} values obtained with the ClogP program (BioByte, 2004) is preferred.

2.1.3.2 K_{oc}

For the selection of the K_{oc} value, experimentally determined values should be retrieved; preferably as much as possible. These K_{oc} values may be derived from standardised tests (e.g. OECD guideline 106; OECD, 2000) or from other studies published in scientific literature. K_{oc} values determined by the HPLC method (OECD guideline 121; OECD, 2001) should be considered as estimates of the real K_{oc} values and consequently, these values are not used as experimental values. Because K_{oc} values may vary widely and no value for K_{oc} can be considered as the most reliable value, the geometric mean of all valid K_{oc} values is calculated, including one value estimated from K_{ow}. This geometric mean K_{oc} will be used as the selected value in ERL derivations (Otte *et al.*, 2001).

2.1.3.3 $K_{p,\ susp\text{-}water}$

For organic substances, the value of $K_{p,\ susp\text{-}water}$ is derived from the K_{oc} value and the fraction organic carbon of suspended matter used within the EU ($Foc_{susp,\ TGD}$), applying Eq. 1. Note that the fraction organic carbon is equal to 0.1 in this case (the EU standard), since the outcome of this equation triggers $MPC_{sediment}$ derivation and should be uniform within Europe.

$$K_{p,\ susp-water} = K_{oc} \times Foc_{susp,\ TGD} \qquad (1)$$

If data for suspended matter are available these can be used directly as well and might be preferred. The value for $K_{p,\ susp\text{-}water}$ for metals is derived from experimental data. From the valid $K_{p,\ susp\text{-}water}$ values summarised in the table containing physicochemical properties (section 2.1.2.6), the geometric mean value is calculated. This geometric mean $K_{p,\ susp\text{-}water}$ will be used as selected value in ERL derivations. If experimental data on K_p for metals are lacking, the data gap is reported and

its possible solution is reported. A solution to this potential problem is outside the scope of this document and should be discussed within the project team dealing with the ERL derivation.

2.1.3.4 Water solubility

The selected value for the water solubility may be calculated from the geometric mean of all valid values for the water solubility. Values below 10 $mg \cdot L^{-1}$ determined with the shake-flask method should be considered as unreliable. For these poorly soluble compounds, the geometric mean of the generator column and slow-stirring is used as selected value.

2.1.3.5 Vapour pressure

In general, the guidance in Table 5 can be used to determine which values for the vapour pressure are reliable. However, if results from different methods deviate significantly from each other, only the methods with a direct analysis of the compound should be used, e.g. the gas saturation method. Complementary to this, the data from GC retention times may be used if there are not enough reliable data. If no experimental data are available, the estimate from EPI Suite can be used (U.S. EPA, 2007b).

2.1.3.6 Henry coefficient

The validity of values for the Henry coefficient should be considered on a case-by-case basis. When no reliable experimental values are available, the Henry coefficient can be estimated from the quotient of the vapour pressure and the water solubility, provided that reliable values are available for both parameters. If this is not the case, the estimate from EPI Suite can be used (U.S. EPA, 2007b).

2.2 Toxicity data

2.2.1 Data collection

To collect toxicity data for a compound the following steps should preferably followed:

1. Contact persons from environmental agencies in other countries are consulted by sending out an e-mail enquiry, in which they are asked if they have access to specific information on toxicity data and/or physicochemical data (see section 2.1.1.2) and are willing to share those data.
2. The industry parties involved in production or use of the compounds under investigation are invited to submit relevant studies, which will be treated as public literature.
3. Thereafter the on-line literature systems Current Contents and TOXLINE are screened.
4. It is important to perform a retrospective literature search. The reference lists of publications or reports obtained should be carefully checked for related studies that have been published at earlier dates. A copy of each study that is deemed relevant should be obtained.
5. The ECOTOX database from the U.S. EPA U.S. EPA, 2007a is searched for relevant ecotoxicological studies. A copy of all studies retrieved from the search results is requested. For RIVM co-workers, the RIVM e-toxBase is also searched for relevant ecotoxicological studies checked by using both CAS number as well the chemical and or common name. The RIVM e-toxBase comprises the U.S. ECOTOX database.
6. The IUCLID database is searched for the compound of interest (European Commission (European Chemical Bureau), 2000).
7. The availability of OECD SIDS documents is checked.
8. The database of the Japanese National Institute of Technology and Evaluation (NITE) is searched for the compound of interest.
9. For pesticides, public assessment reports are available online at several locations. Check the following websites (we do not aim for completeness in the following list):
   UK Pesticides Safety Directorate (PSD): http://www.pesticides.gov.uk/psd_evaluation_all.asp,

US EPA: http://www.epa.gov/pesticides/reregistration/
Health Canada: http://www.pmra-arla.gc.ca/english/pubs/reeval-e.html.

10. A further search is performed in libraries such as the library of the Expertise Centre for Substances (SEC) and the RIVM library.
11. If no or very few data are found in the steps described above, an additional internet search can be performed on the chemical name and CAS number of the compound using established search engines.

In principle, all ecotoxicological studies are evaluated for usefulness in ERL derivation. Studies from which one of the endpoints LC50, EC50, LC10, EC10 or NOEC can be calculated using data presented by the author(s) are also used. Studies that show results in a graph of good quality that might be converted back into raw data are also evaluated.

Ecotoxicity studies conducted in all compartments are searched for: freshwater, seawater, brackish water, groundwater (usually no data), soil, sediment and air. Whether or not data on secondary poisoning should be collected is dependent on some trigger values. These trigger values are discussed in section 3.1.1 for the aquatic compartment and section 3.3.1 for the terrestrial compartment. In the case that secondary poisoning should be assessed, toxicity data for birds and mammals should be collected, screening the appropriate sources described above. In the case of toxicity to birds, acute 5-day studies generating LD50 values should be collected too.

2.2.2 Data evaluation and data tables

An outline of the general procedure of the evaluation of the toxicity data is given below.

1. All retrieved literature is read and evaluated with respect to its usefulness and reliability.
2. Each study should be assigned a quality code. See section 2.2.2.1 for more detail.
3. After evaluating a study, the results of the study are summarised by entering it into the appropriate data table (see sections 2.2.3 and 2.2.4).
   - For aquatic toxicity data, the data on freshwater organisms and data on marine organisms are placed in separate tables.
   - The terrestrial toxicity data are divided into toxicity data on terrestrial species and data on terrestrial microbial processes and enzymatic reactions.
   - Data on aquatic, terrestrial, and benthic species are separated into acute and chronic data, with a separate table for each category (see section 2.2.2.1 for more guidance).
   - Toxicity data on birds and mammals are placed in separate tables. If many data are available, a distinction can be made between studies with oral (gavage) and dietary (food) exposure.
4. Each row of the toxicity data table contains a test result for one species, endpoint and criterion. The columns of the toxicity data table contain the various study parameters. Columns should be filled as completely as possible. When there is no value for a given parameter, the table cell is left empty.
5. All references of toxicity studies mentioned in all toxicity data tables should be included in one or more reference lists.
6. In the toxicity data tables, all tested species are clustered in taxonomic groups, see sections 2.2.3.1 and 2.2.4.1. The taxonomic classification used within the project is given in Chapter 5 and should be followed in all ERL derivations.
7. For terrestrial and benthic toxicity data for organic compounds, recalculate toxicity test results to standard soil or sediment with an organic matter content of 10%. For the procedure, see section 2.2.4.15. In the toxicity data tables on terrestrial and benthic data, both the test result in the test soil or sediment (expressed as a dry weight concentration) as well as the test result in

standard soil (expressed as a dry weight concentration) are reported. For metals, tests can be normalised to standard soil and sediment, with use of both organic matter and lutum content of the soil or sediment. However, the merit of this normalisation for metals is under discussion (section 2.2.4.15).

8. Finally, a new table of selected toxicity data is created in which toxicity data are aggregated to one toxicity value per species. Such a table is created for all compartments. The table will contain the data that are used for the actual risk limit derivation. The guidance to compile this table is given in section 2.2.6.

2.2.2.1 Study quality: validity codes

The scoring system that is followed is that developed by Klimisch *et al*. (1997). The quality codes assigned are:

1 = reliable without restrictions: 'studies or data...generated according to generally valid and/or internationally accepted testing guidelines (preferably performed according to GLP) or in which the test parameters documented are based on a specific (national) testing guideline...or in which all parameters described are closely related/comparable to a guideline method.'

2 = reliable with restrictions: 'studies or data...(mostly not performed according to GLP), in which the test parameters documented do not totally comply with the specific testing guideline, but are sufficient to accept the data or in which investigations are described which cannot be subsumed under a testing guideline, but which are nevertheless well documented and scientifically acceptable.'

3 = not reliable: 'studies or data...in which there were interferences between the measuring system and the test substance or in which organisms/test systems were used which are not relevant in relation to the exposure (e.g., unphysiologic pathways of application) or which were carried out or generated according to a method which is not acceptable, the documentation of which is not sufficient for assessment and which is not convincing for an expert judgment.'

4 = not assignable: 'studies or data....which do not give sufficient experimental details and which are only listed in short abstracts or secondary literature (books, reviews, etc.).'

- In general, when a test has fundamental shortcomings, it should be classified as not reliable (3). This applies to situations where the test was incubated too long (e.g. for algae) or too wet (for soil), the oxygen content was too low, control mortality was too high, solubility of the test substance was exceeded (see section 2.2.2.3 for more detail), a co-solvent or emulsifier has been used in high concentrations (see section 2.2.2.4), pH was out of the appropriate range (see section 2.2.2.5 for specific guidance), the light used had an unrealistic UV-intensity, the identity of the substance is not clear (see section 2.2.2.6 for more guidance), or tests for which the actual concentrations are largely unknown due to significant but not quantified loss, etc.
- If the experiment is carried out in a medium that is not the natural habitat of the tested species, these tests are generally not reported rather than being classified as not reliable (see section 2.2.2.7 for more guidance).
- When a study contains useful toxicity information but it can not be used directly for derivation of ERLs, it is still tabulated. Examples are a NOEC value from a short term test, or a value higher than the highest tested concentration or lower than lowest tested concentration (see section 2.2.2.8 for more detail). The test can then still be classified as reliable or reliable with restrictions.

2.2.2.2 Acute and chronic studies

Within the INS framework, a chronic toxicity study is defined as a study in which:

(i) the species is exposed to the toxicant for at least one complete life cycle, or
(ii) the species is exposed to the toxicant during one or more sensitive life stages.

This definition is in line with the TGD and the FHI document, which state that NOECs from chronic/long-term studies should preferably be derived from full life-cycle or multi-generation studies. In the TGD, it is made clear that true chronic studies cover all sensitive life stages. Unfortunately, no clear guidance is provided on individual studies, whether these are to be considered as chronic studies or as acute studies. What is considered chronic or acute is very much dependent on 1) the species considered and 2) the studied endpoint and reported criterion.

With regard to the most common species, toxicity studies with fish are considered acute if mortality is considered after 96 hours (standard acute test) or after 14 days (prolonged acute toxicity test). The most common chronic toxicity tests for fish are early life-stage tests (ELS), in which eggs or larvae are exposed and the effects on hatching, malformation and growth are considered. Most ELS tests for fish, but also for other species such as amphibians (FETAX test) or echinoderms, can be considered as chronic toxicity studies (see also TGD, page 186). For daphnids, the standard exposure time for acute toxicity is 48 hours, but with regard to chronic toxicity, there is a factor of three difference between the tests with *Daphnia magna* (21 days) and *Ceriodaphnia dubia* (7 days), the latter having a much shorter reproduction time. For algae, the standard exposure time is 72 hours. In this time, the algae regenerate several times. However, the EC50 of this test is considered as acute, while the NOEC or EC10 of such test is a chronic value (TGD).

2.2.2.3 Comparison of toxicity value with water solubility

In principle, toxicity studies that have been conducted at concentrations above the water solubility should not be used in the risk assessment. However, depending on the uncertainty in the estimate of the water solubility, test results (L(E)C50, NOEC, EC10) that are ≤ 2 times the estimated value might be included in the risk assessment. The factor of 2 is a rather arbitrary value; when experimental data show that the variation in the estimate of the water solubility is lower, it should be lowered accordingly. When the variation in the estimate of the water solubility is higher than a factor of 2, it may be increased to a factor of 3 (maximum). Toxicity studies showing results above the water solubility receive a footnote stating: ‘test result above water solubility’.

2.2.2.4 Use of co-solvents, emulsifiers and dispersants

Sometimes, the solubility of a compound is so low that a solvent, emulsifier or dispersant is used to prepare suitably concentrated stock solutions of the test substances. Such vehicles may not be used to enhance the solubility of the test substance in the test medium, and in any case the compounds used for this purpose may not be toxic to the tested species. Therefore, a control with the vehicle (solvent control) used should be incorporated in the set-up of the test. According to several OECD test guidelines for aquatic toxicity testing (see section 2.2.2.10) the concentrations of the solvent, emulsifier or dispersant should not exceed 100 $mg.L^{-1}$ (or 100 $\mu l.L^{-1}$ or 0.01%).

2.2.2.5 pH of test water and pK_a and ionisation of test compound

When a test has been performed according to a guideline, the pH should be within the required range and, if not, it should be checked whether the test can be considered valid. Expert judgement should be employed to determine if a test result should be excluded. A test may become invalid because the test organisms naturally occur at other pH values.

In some cases, the compound itself may alter the pH strongly. In such cases, it should always be checked whether the observed toxicity might be caused by this change in pH. If so, the test must be

considered as invalid, because the buffering capacity of the environment will prevent such a pH effect in the field. For compounds containing functional groups with acidic or basic properties, the pK_a value(s) should be reported in the table with physicochemical properties (section 2.1.2). Attention should be paid to possible relationships between pH and toxicity of the tested compound, for example, due to a reduced availability (speciation, precipitation, hydrolysis, etc.) of the test compound. The toxicity of a compound may be influenced by its degree of ionisation[7]. As a rule, hydrophobicity, and consequently bioaccumulation and toxicity, of a given compound are expected to increase with decreasing degree of ionisation. In other words: the higher the proportion of neutral molecules, the higher the toxicity. The degree of ionisation of a compound in a toxicity test is determined by several factors:

- the pK_a (s) of the test compound,
- the concentration of the test compound,
- pH of the test compartment (soil, water, sediment),
- the buffering capacity of the test-matrix.

In practice:

1. a compound's potential to ionise (pK_a in physicochemical table) should be checked;
2. presence of one or more pK_a value(s), or ionisable group(s), triggers the attention for pH effects in toxicity studies;
3. if toxicity test results reveal that toxicity is dependent on the pH of the test-matrix (soil, water, sediment), it might be considered to reject test results if the pH falls outside the range of what can be expected naturally.

Test results should be rejected when it can be inferred that the toxicity in a given study is not caused by the compound alone, but also by a pH change. Hence, results from tests with ionisable compounds performed in buffered media (providing sufficient buffering capacity) may be considered more reliable than those performed without a buffer. Those studies that explicitly mention a measured pH after addition of the toxicant are most useful in this respect.

2.2.2.6 Purity and identity of the test substance

In some tests the identity of the test substance is largely unknown or the purity of the test substance is very low. Depending on the nature of the impurities present, if these have been identified at all, a minimum purity of 80% is required, unless it is known that the impurities do not cause any toxic effects by themselves and do not influence the toxicity of the substance of interest. When the purity of the tested compound is < 90%, the test result should be corrected for purity. For technical mixtures of compounds of which a substantial fraction (impurity) consists of one or more compounds structurally related to the test compound, it is subject to expert judgement whether the test result is useful for risk limit derivation or not.

2.2.2.7 Toxicity studies performed in other media

- If the study is performed in a medium that is not representative for the tested species, for example, terrestrial plant toxicity studies that were conducted in nutrient solution or toxicity studies with earthworms on filter paper, these studies are not further evaluated. Effect concentrations for terrestrial species should be expressed in weight units per kg soil, and this is impossible when a study was conducted in water or filter paper. These types of tests may be used for purposes of comparison. Terrestrial species tested in nutrient solution can be compared with aquatic species if equilibrium partitioning is used to derive the environmental risk limits for soil. However, generally these studies in nutrient solution are not reported.

[7] 'Degree of ionisation' as used in this section expresses the ratio of the number of charged molecules over the total number of neutral and charged molecules at a given concentration and at a given pH.

- In some terrestrial toxicity studies, concentrations in pore water are reported. Results from these studies can only be used if truly dissolved concentrations have been measured (e.g. by SPME or SPMD techniques). Analyses in pore water obtained after centrifugation are not useful in this respect. Equilibrium partitioning should be applied to the pore water concentration, in order to calculate a concentration in soil that can be used in ERL derivation.
- Benthic species are often tested in a water-only system. In such cases the data are still tabulated. However, it should be assessed as to what extent it is plausible that the organisms are exposed via the water phase. For organisms that are living in the sediment and not on the surface of the sediment, these tests should be assigned the code 'invalid'.

2.2.2.8 Dealing with toxicity values higher or lower than range of test concentrations

If the highest concentration in a toxicity test is not high enough to determine the NOEC or L(E)C50, the result of that study should be tabulated as NOEC ≥ or L(E)C50 >, followed by the value of the highest test concentration. The test result should be reported in the toxicity data tables.
The result itself is not used in calculations of risk limits. However, it is valuable information that a species from this taxon (or trophic level) has been tested and that it was not sensitive to the toxicant at a known concentration. This applies specifically to the case of limited data sets. For example: when NOEC values for algae, *Daphnia* and fish are found, of which one is a 'NOEC ≥ ' value, and this value is not the lowest effect concentration, an assessment factor of 10 may be applied, whereas this would have been 50 if the study had been rejected.

For similar reasons, the data from tests resulting in an effect at the lowest test concentration should be tabulated as NOEC < or L(E)C50 <, followed by the value of the lowest test concentration. Although these values can not be used directly for the derivation of the risk limits, useful information can be derived from the comparison of the sensitivity of that specific species with the derived risk limit. This comparison may facilitate the decision for the final assessment factor that is applied for the derivation of the risk limit.

2.2.2.9 Quality criteria and GLP criteria

In this report, a list of criteria that determine whether a study is acceptable or unacceptable for ERL derivation, is not given. The decision to accept or to reject a toxicity study for use in ERL derivation is based on expert judgment. Additionally, all reports published within the INS framework are reviewed by one or more expert(s) in the field and peer-reviewed by the scientific sounding board INS.

In the field of ERL derivation, toxicity studies originate from various sources, which are tracked as much as possible to the original source. The two key sources are (i) publications in scientific journals and (ii) original study reports that have not been published elsewhere. It must be stated that up till now the latter category has been in the minority, since for reasons of confidentiality, original study reports are often unpublished and inaccessible.

Studies conducted by researchers from laboratories that work according to procedures embedded in a laboratory specific quality assurance framework, e.g. Good Laboratory Practice (GLP), are deemed equally relevant to those studies that are conducted by researchers from laboratories that do not work according to such frameworks or have not reported this. For ERL derivation, it is important to realise that all studies are to be evaluated without an *a priori* judgment with respect to quality. The set-up and the description of a study and, if possible, comparison with results from comparable studies and organisms, should provide all information necessary to assess its quality.

2.2.2.10 Use of toxicity tests performed according to established guidelines

For several toxicity studies with different species, international guidelines exist for performing these studies. If such protocols are followed and the requirements for the study are met, the results from such studies are very useful in the derivation of the environmental risk limits. The most important guidelines for ecotoxicological studies are summarised in this section. It is indicated how to deal with the results for each study.

- OECD guideline 201: Alga, Growth Inhibition Test. The EC50 from this 72-h algae test is considered an acute value, the NOEC or EC10 a chronic value.
  The guideline version from 1984 mentions both biomass (sometimes called growth) and growth rate as endpoints. From studies based on the OECD 201 - 1984 guideline, the value for the growth rate is preferred, because this is the more relevant parameter (European Commission (Joint Research Centre), 2003a). However, if only growth is presented, this value can be used as well. The result for the endpoint biomass (growth) is generally somewhat lower than the growth rate and can therefore be considered as a conservative value.
  N.B. This guideline was revised in 2006. Endpoints derived from a study conducted following the revised (2006) are both valid.
- OECD guideline 202: *Daphnia* sp., Acute Immobilisation Test. For the derivation of the risk limits for water only the EC50 from this 48-h acute toxicity study is considered. The endpoint is immobility, as indicated by the inability to swim after agitation.
- OECD guideline 203: Fish, Acute Toxicity Test. For the derivation of the risk limits for water only the LC50 from this 96-h acute toxicity study is considered. The recorded endpoint is mortality.
- OECD guideline 204: Fish, Prolonged Toxicity Test: 14-day Study. This study is also considered as an acute toxicity study, and consequently, in most cases, only the LC50 is used for the derivation of environmental risk limits.
- OECD guideline 205: Avian Dietary Toxicity Test. This test can be used as an acute toxicity test with birds for the assessment of secondary poisoning.
- OECD guideline 206: Avian Reproduction Test. This test can be used as a chronic toxicity test with birds for the assessment of secondary poisoning, because the exposure duration is at least 20 weeks.
- OECD guideline 207: Earthworm, Acute Toxicity Tests. This test can be used as an acute test. The endpoint is mortality.
- OECD guideline 208: Terrestrial Plants, Growth Test. According to the test guideline the recorded endpoints should be the LC50 for emergence and the EC50 for growth. As such, the test is an acute test. However, because exposure is from seed to plant, the test may be interpreted as chronic if NOECs or EC10s are recorded for the above mentioned endpoints, especially if the exposure duration is prolonged to, for example, 28 days.
- OECD guideline 210: Fish, Early-life Stage Toxicity Test. This test with fish is a chronic test which covers the life cycle of fish from eggs to free feeding juvenile fish. The recorded endpoints are mortality at all stages, time to hatch, hatching success, length, weight and any morphological or behavioural abnormalities.
- OECD guideline 211: *Daphnia magna* Reproduction Test. This is a chronic test with water fleas. The most important endpoint is the number of young per female (both young and parent alive). Other endpoints are the survival of the parent animals and time to production of first brood. Additionally, parameters such as growth (e.g. length) of the parent animals, and possibly intrinsic rate of increase are useful endpoints.
- OECD guideline 212: Fish, Short-term Toxicity Test on Embryo and Sac-fry Stages. In the guideline it is stated that this test can be used as a screening test for chronic toxicity.

Especially for species that can not be kept under laboratory circumstances for a period long enough to perform a full early-life stage (ELS) test, this test can be a useful alternative. Because the sensitive life stages from egg to sac-fry are covered in this test, it can be considered a chronic test. However, it is expected to be less sensitive than the full ELS test. The same endpoints are recorded as for the full ELS test.

- OECD guideline 215: Fish, Juvenile Growth Test. Because the recorded endpoint is growth during 28 days and the criterion is the NOEC or EC10, the test can be regarded as chronic.
- OECD guideline 216: Soil Micro organisms: Nitrogen Transformation Test. This 28-d test is a chronic test for microbial processes. It is useful, provided that the NOEC or EC10 is reported or can be calculated.
- OECD guideline 217: Soil Micro organisms: Carbon Transformation Test. The same as for the OECD guideline 216 applies to this test guideline.
- OECD guideline 218: Sediment-Water Chironomid Toxicity Test Using Spiked Sediment. This is a chronic toxicity study with a chironomid species. The measured endpoints are the total number of adults emerged and the time to emergence. Additionally, larval survival and growth after a ten-day period are recommended endpoints.
- OECD guideline 219: Sediment-Water Chironomid Toxicity Test Using Spiked Water. This test is similar to OECD guideline 218. However, for reasons of stability of the test concentrations, the OECD 218 is preferred. If a test with spiked water is available this test should always be accompanied by a determination of actual concentrations in the sediment.
- OECD guideline 220: Enchytraeid Reproduction Test. The 14-d range finding test from this guideline in which mortality is recorded is an acute test. The definitive test that lasts for 6 weeks is a chronic test. In this test the number of offspring is recorded as well as the mortality of the parent animals, which are only exposed for three weeks and are thereafter removed from the system.
- OECD Revised Proposal for a New Guideline 221: *Lemna* sp. Growth Inhibition Test. For this 7-d test with duckweed the same considerations can be made as for the algal test (OECD 201): the EC50 from this test is considered an acute value, the NOEC or EC10 a chronic value. Both chronic and acute data should be retrieved from the test. The preferred endpoints are growth rate (based on frond number) or biomass (dry weight, fresh weight or frond area).
- OECD guideline 222: Earthworm Reproduction Test (*Eisenia fetida* / *Eisenia andrei*). This test is similar to the chronic reproduction test with enchytraeids (OECD guideline 220). However, in this test the parent worms are exposed for 4 weeks and the reproductive output is assessed after another 4 weeks.
- FETAX (Frog Embryo Teratogenesis Assay *Xenopus*): This test is a rather short test of 96 hours duration, possibly extended with a few hours, if the larvae have not reached a certain developmental stage. However, considering the sensitive endpoints (next to mortality also development and malformation) and the sensitive life stage (embryonic stages), this test can be considered as chronic for the derivation of environmental risk limits.
- EPA. Ecological Effects Test Guidelines. OPPTS 850.1735. Whole sediment acute toxicity invertebrates, freshwater. Draft, 1996. This test can be used as a chronic test for species such as *Hyalella azteca*.

Next to the tests on birds (OECD guidelines 205 and 206), the OECD has a series of guidelines of toxicity tests with mammals for use in the human health risk assessment. These data might be used in the derivation of the environmental risk limits based on secondary poisoning as well, provided that only those effects are selected that relate to the effects at the population level of the species. The following OECD guidelines are most important in this respect:

- OECD guideline 401: Acute Oral Toxicity
- OECD guideline 407: Repeated Dose 28-day Oral Toxicity Study in Rodents
- OECD guideline 408: Repeated Dose 90-Day Oral Toxicity Study in Rodents
- OECD guideline 409: Repeated Dose 90-Day Oral Toxicity Study in Non-Rodents
- OECD guideline 414: Prenatal Development Toxicity Study
- OECD guideline 415: One-Generation Reproduction Toxicity Study
- OECD guideline 416: Two-Generation Reproduction Toxicity

2.2.3 Aquatic toxicity data tables

The following sections (2.2.3.1 to 2.2.3.18) discuss the parameters that are reported in the aquatic toxicity data tables for acute, chronic, freshwater and marine data. The aim is to fill the table as complete as possible. The parameters are treated in the same order as they appear in the default toxicity data table. The following subsections have titles identical to the column titles in the data tables. Part of the text in this chapter is cited from Traas (2001).

2.2.3.1 Species

All available toxicity data for a given compound are ordered by test organism. Species are grouped in taxonomic subsections. A comprehensive list of taxonomic groups discerned within the INS framework is shown in Chapter 6. Both taxa and species names are reported in Latin. Taxonomic groups are shown in bold font, species names are shown in italic font. Species names within a taxon are listed in alphabetical order. For example:

Bacteria
Pseudomonas putida

Algae
Chlorella vulgaris
Pseudokirchneriella subcapitata
Scenedesmus acuminatus

Crustacea
Daphnia pulex

2.2.3.2 Species properties

The most relevant properties of the test organism are mentioned in this column; e.g. age, size, weight, life stage or larval stage. Toxicity data for organisms with different age, size, life stage etc., are presented as individual entries (i.e. one entry in each row) in the data table.

2.2.3.3 Analysed

This column reports whether the test compound is analysed during the experiment. Y (Yes) is entered in this column, when the compound has been analysed. When no analysis for the test compound is performed, N (No) is entered in this column.
In some cases the test compound is analysed, but the test results (L(E)C50, EC10, NOEC) are not calculated from the actual concentrations. If the test result is based on nominal concentrations, this is mentioned in a footnote to this study: ‘Test result based on nominal concentrations’. When this is valid because measured concentrations are close to initial concentrations (drop in concentration < 20% over exposure period), ‘Test result based on nominal concentrations, measured concentrations were > 80% of nominal’ is noted.
If the test compound is analysed but not used for the test results and there is considerable change in the concentration during the test (> 20% loss of test compound), the test result is recalculated using

actual concentrations. In such case, in a footnote to this study should be mentioned that tests results were recalculated to actual concentrations.

When, in static or renewal tests, samples are analysed at different points of time, the mean of the measured values is used. When the initial concentration is not measured and one or more samples during the test are, a mean of the initial nominal and the measured concentration(s) is used. In general, taking the average of start and end concentrations slightly overestimates the average concentration during the whole experiment, while the geometric mean underestimates the concentration. For calculating the mean concentration during the course of a static experiment, the best assumption is an exponential decay of the concentration in time. In continuous flow experiments, the concentrations are usually reported as mean measured values, and here, no further calculations are necessary.

2.2.3.4 Test type

The following test types are distinguished:

S	static system
Sc	static system in closed bottles or test vessels
R	renewal system (semi-static)
F	flow-through system
CF	continuous flow system
IF	intermittent flow system

2.2.3.5 Test compound

- This column can be deleted when the compound under consideration has only one structural molecular configuration.
- If the tested compound is a metal, the tested metal salt should be reported here.
- If the tested compound is a stereoisomer[8], consists of a mixture of isomers, etc., the name of the tested molecule(s) should be reported here. For some stereo-isomers it might be preferred to derive individual risk limits. The stereoisomers dieldrin and endrin are an example of such a case.
- If the tested compound is a structural isomer, the individual compounds, in general, have different physicochemical and toxicological properties and each compound will be subject of an ERL derivation (see next paragraph).
- Formulated products (e.g. biocides, pesticides)

Structural isomers

Compounds that are structural isomers are, in principle, regarded as different compounds, e.g. ethanol and dimethyl ether or anthracene and phenanthrene. In these cases, each individual isomer will generally be the subject of an ERL derivation. As a rule of thumb, within the INS framework, isomers can be regarded as individual compounds when they have different CAS registry numbers. However, for more complex molecules[9] consultation with an expert or the client (e.g. the Ministry) might be needed.

2.2.3.6 Purity

Unit: %

[8] Stereoisomers: geometric isomers (*cis*- and *trans*-isomers or E- and Z-isomers), optical isomers (+ and – isomers or R- and S-isomers) and conformational isomers (e.g. chair and boat structures in cyclohexane ring structures).

[9] Isomers might be distinguished by CAS nos., but still be treated (generally) as ‘one compound’, e.g. ‘nonylphenol’. The nonyl chain can have many conformations and different CAS nos. exist. However, the generic name ‘nonylphenol’ is mostly used for all *para*-nonylphenol isomers.

The purity of the test compound expressed as percentage is reported in this column. Alternatively, the following abbreviations may be entered for the designation of chemical purity.

ag	analytical grade
lg	laboratory grade
pa	pro analyse
rg	reagent grade
tg	technical grade

Here, the first four have a relatively high purity, while technical grade is in general somewhat less pure. When the purity of the test compound is expressed only by an abbreviation, this abbreviation is reported. However, a purity expressed as percentage is preferred.

2.2.3.7 Test water

In this column, the test water or medium is reported using abbreviations. Choose from the following list. A footnote to the test may be added if further description of the test medium is needed.

am	artificial medium, such as media used for bacterial and algal tests, artificial seawater
dtw	dechlorinated tap water
dw	de-ionised water, dechlorinated water or distilled water
nw	natural water, such as lake water, river water, sea water, well water
rw	reconstituted water: (natural) water with additional salts
rtw	reconstituted tap water: tap water with additional salts
tw	tap water

2.2.3.8 pH

If possible, measured pH values should be reported. If a pH range is given, this range is reported.

2.2.3.9 Temperature

Unit: °C

In this column the temperature at which the test is performed should be reported, preferably a measured temperature. If a temperature range is given, the range is reported.

2.2.3.10 Hardness

Unit: mg $CaCO_3.L^{-1}$

This column is shown in tables showing data from freshwater experiments, not for marine water. The hardness of the test water should be reported here. If the hardness of an artificial medium is not reported, but the composition of the medium is reported, the hardness should be calculated. Recalculation should be performed by summing the molar concentrations of all calcium (Ca) and magnesium (Mg) salts and expressing the result as $CaCO_3$ in units of $mg.L^{-1}$.

2.2.3.11 Salinity

Unit: ‰

This column is only shown in tables showing data from saltwater experiments, and takes the place of the column for hardness in the freshwater tables. The salinity of the test water should be presented here. A practical definition of salinity[10] is based on the weight of the eleven most abundant components present in one kg of seawater. In practice it may also be determined by recalculating the measured chloride ion only to total salinity, using the assumption that the total amount of all components in the oceans is constant. The average salinity of seawater is around 35‰, which roughly equals 35 g of salts per kg (one litre) of seawater. The unit of salinity might also be found expressed in promille or ppt, i.e. parts per *thousand* (not parts per trillion in this case) as w/w. To derive the salinity expressed in promilles the following conversion can be applied:

– when only chloride ions (Cl^-) have been measured, the salinity can be recalculated to ‰ from the chloride concentration using: S(ppt) = 1.80655 × chloride concentration (ppt), in which S = salinity
– psu = practical salinity units[11]. One psu roughly equals one ppt (‰). Seawater has a salinity of approximately 35 psu ≈ 35 ‰ = 35 $g.kg^{-1}$.

Animals living (and tested) in brackish water environments are not placed in separate tables, but are included in the saltwater tables. The division between freshwater, brackish water and seawater on basis of salinity is given in Table 8. The division in these categories is rather arbitrary and depends on the source used. For the division between freshwater and brackish water, 0.5‰ and 5‰ are mentioned. The latter value was formerly used within INS framework (Traas, 2001), but the value of 0.5‰ is as such defined in the Water Framework Directive (European Commission, 2000). Consequently, the value of 0.5‰ will be used in the INS framework. Moreover, typical freshwater in the Netherlands has salinity in the range of less than 0.5‰ and many freshwater organisms adversely affected by higher salinities. Also for the division between brackish water and seawater several values for the salinity can be found. Because brackish water and seawater are treated together, this division is less relevant. However, toxicity tests in brackish water performed at relatively low salinity (e.g. less than the 5‰) might be less relevant for the marine environment as well.

Table 8: Classification of water according to salinity.

Water type	Salinity (‰)
freshwater	<0.5
brackish water	0.5 – 30
seawater	30 – 40

2.2.3.12 Exposure time

The duration of exposure to the toxicant in the toxicity experiment is expressed in this column. The abbreviations listed below in Table 9 can be used. The last column gives an indication of which unit of time to use at which exposure duration. A rule of thumb is to stick to the most common expression of test duration in case of standardised tests (e.g. OECD or ISO tests) where this is possible. For example, for a reproduction study with *Eisenia fetida* 56 days is noted rather than ‘1.8 months’.

[10] The most recent definition of salinity is based on the ratio of electrical conductivity of seawater at standard conditions to that of a KCl solution at standard conditions. This method yields a salinity expressed in practical salinity units (psu).
[11] However, due to the qualitative nature in which salinity is used in ERL derivation, this definition and its inherent accuracy are not relevant to the INS framework.

Table 9: Used abbreviation and applied range for exposure times.

Test duration in	Abbreviation	Duration
minutes	min	0-60 minutes
hours	H	1-120 hours
days	d	5-56 days
weeks	w	1-4 weeks
months	mo	1-12 months
years	y	≥ 1 years

2.2.3.13 Criterion

The criteria commonly encountered in ecotoxicological tests are summarised in Table 10. Their use (or not) in ERL derivation is described in columns 3 and 4 of this table. For explanation of abbreviations please see the List of abbreviations at page 129.

Table 10. Criteria derived from toxicity studies and their use in ERL derivation – summary.

Test type	**Criterion**	**Use in ERL derivation?**	**Action**
acute test	EC10 or LC10	No [a]	▪ Tabulate value; may be valuable as additional information
acute test	EC50 or LC50	Yes	▪ Tabulate value
acute test	ECx or LCx	No	▪ Tabulate value; may be valuable as additional information
acute test	LOEC	No	▪ Omit if NOEC is also available from same experiment ▪ Else: tabulate value; may be valuable as additional information
acute test	MATC[12]	No	▪ Omit if NOEC is also available from same experiment ▪ Else: tabulate value; may be valuable as additional information
acute test	NOEC	No [a]	▪ Tabulate value; may be valuable as additional information
acute test	TLm	Yes	▪ Tabulate as LC50 [b]
chronic test	EC10 or LC10	Yes	▪ Tabulate value
chronic test	EC50 or LC50	No [a]	▪ Tabulate value; may be valuable as additional information
chronic test	ECx (x < 10)	No	▪ Omit if NOEC is also available from same experiment ▪ If more than one ECx value is available, try to establish an EC10 from a reliable dose-response relationship ▪ Else: tabulate value; may be valuable as additional information
chronic test	ECx (10 < x < 20)	Yes	▪ Omit if NOEC is also available from same experiment ▪ If more than one ECx value is available, try to establish an EC10 from a reliable dose-response relationship ▪ Tabulate value if the ECx is the lowest effect concentration measured. Calculate NOEC = ECx/2 (TGD guidance) and tabulate this NOEC [c]
chronic test	ECx (x ≥ 20)	No	▪ Tabulate value; may be valuable as additional information ▪ If more than one ECx value is available, try to establish an EC10 from a reliable dose-response relationship
chronic test	LOEC	No	▪ Omit if NOEC is also available from same experiment ▪ Else: (i) if percentage effect is known, see ECx in this table for further guidance ▪ Else: (ii) if percentage effect is unknown: tabulate value; may be valuable as additional information
chronic test	MATC - single value, no further information	Yes	▪ Omit if NOEC is also available from same experiment ▪ Else, if no further information is available, calculate NOEC = MATC/√2 (TGD guidance) and tabulate this NOEC [d]

[12] The MATC is the geometric mean of NOEC and LOEC.

Test type	Criterion	Use in ERL derivation?	Action
chronic test	MATC - reported as a range	Yes	▪ Omit if NOEC is also available from same experiment ▪ Else, if no further information is available, tabulate the lowest value of the range as NOEC [e]
chronic test	MATC – spacing factor is given [f]	Yes	▪ Omit if NOEC is also available from same experiment ▪ Else, if no further information is available, calculate NOEC = MATC/√(spacing factor)[f] and tabulate this NOEC [g]
chronic test	NOEC	Yes	▪ Omit LOEC if it is also available from same experiment

Notes to Table 10.

a) For toxicity tests with algae and *Lemna* sp., both the EC50 and the EC10 or NOEC are used in the ERL derivation, if available.
b) A footnote should be added to the toxicity data table stating that the TLm is used as LC50.
c) A footnote should be added to the toxicity data table stating that the NOEC is calculated as ECx/2.
d) A footnote should be added to the toxicity data table stating that the NOEC is calculated as MATC/√2.
e) A footnote should be added to the toxicity data table stating that the lowest value of the MATC range is taken as NOEC.
f) The spacing factor is the factor of difference between two subsequent testing concentrations employed in the toxicity experiment.
g) A footnote should be added to the toxicity data table stating that the NOEC is calculated as MATC/√(spacing factor).

Additional information to Table 10

The most common criteria are either EC50 or LC50 in the case of acute toxicity tests and EC10 or NOEC in the case of a chronic test. Other examples of criteria that are regularly found in the literature are LOEC, MATC, which is the geometric mean of NOEC and LOEC, and TLm, which is equivalent to the LC50.

If a NOEC is reported, the LOEC can be omitted. In general, EC50 and LC50 values are used from acute studies and NOEC and EC10 (ECx) values from chronic studies. For reasons of completeness and as supporting information for the derivation of the ERLs, EC50 and LC50 values from chronic studies as well as NOEC and EC10 values from acute studies may be documented in the data tables.

If the endpoint presented is an ECx or LOEC value with an effect between 10 and 20%, then a NOEC can be derived according to the TGD, by dividing the ECx by a factor of 2. In such a case, the NOEC can be presented in the toxicity data table, with a note that this value is estimated from an ECx value.

In a strict sense, calculating NOEC as ECx/2, according to the TGD, is only allowed for ECx values with an effect smaller than 20%. However, EC20 values are often presented in the literature. If there is no other information on the dose-response relationship (e.g. a companion EC50, which enables the calculation of an EC10), the EC20 divided by 2 can be considered as NOEC as well, accompanied by a footnote in the table with selected toxicity data (see section 2.2.6).

However, in all cases, the information on a dose-response relationship must be used as much as possible. If it is possible to derive EC50 and EC10 values from a range of tabulated or graphically presented ECx values, these derived endpoints can be included in the toxicity data table as well, accompanied by a footnote stating the method of derivation.

2.2.3.14 Test endpoint

The toxicological parameter for which the test result is obtained is tabulated here. The list below shows some relevant endpoints:

growth (weight, length, growth rate, biomass)

number (cells, population)
mortality
immobilisation
reproduction
hatching (rate, time, percentage)
sex ratio
development (egg, embryo, life stage)
malformations (teratogenicity)
proliferation (cells)
filtration rate
carbon uptake (algae)
reburial (of e.g. certain crustacean species)

This list gives some examples, but it should be noted that it is surely not exhaustive. In general only those endpoints are considered that have consequences at the population level of the test species (see section 2.2.6). Toxicity test results based on endpoints of which the relationship to effects at the population level is uncertain or not established, are not included in the toxicity data tables. Some examples are:

blood or plasma protein levels
histopathological endpoints
organ weights (e.g. hepatosomatic index, gonadosomatic index)
mRNA induction
endpoints determined *in vitro* tests
behavioural responses (e.g. swimming behaviour, antenna motility, etc.)
coloration

Note however, that the use of these types of endpoints for ERL derivation might be reconsidered when a definite correlation or causal relationship with an effect at the population level is established.

2.2.3.15 Value

Unit: $mg.L^{-1}$, $\mu g.L^{-1}$.
The unit in which the results of toxicity tests are expressed is optional. For reasons of comparison and to avoid errors, the same unit is used throughout all aquatic toxicity data tables in one report. In general, values are expressed in two or three digits. At most, four significant digits are reported. However, further calculation with these data may be necessary: averaging, dividing the values by an assessment factor, use of the results in SSDs, etc. Further calculation is always performed with the original (*not rounded off*) values.

Toxicity data of metal compounds are always expressed in quantities of the element, not as the salt. For example, a test performed with $CoSO_4.7H_2O$ is expressed as Co^{2+}. Test results are recalculated if necessary. A similar approach is followed for all charged substances with a non-toxic counter ion.

2.2.3.16 Validity

This column contains a number (1, 2, 3 or 4), indicating the quality of the study summarised. Section 2.2.2.1 describes the background of the quality scoring system.

2.2.3.17 Notes

This column contains references to footnotes that are listed below the toxicity data tables. Numbers are used to refer to footnotes.

2.2.3.18 Reference

The reference to the study from which data are tabulated has the following format:

1 author	Bringmann, 1956
2 authors	Bringmann and Kühn, 1976
3 or more authors	Bringmann *et al*., 1977

If two or more studies have the same citation, distinguish between the different studies by adding a character to the year, e.g. 1980a. All cited references are listed in a reference list.

2.2.4 Terrestrial and sediment toxicity data tables

The following sections (2.2.4.1 to 2.2.4.18) discuss the parameters that are reported in the toxicity data tables on acute and chronic toxicity data for terrestrial and benthic species and on terrestrial microbial processes and enzymatic reactions. The aim is to fill in the table as completely as possible. The parameters are treated in the same order as they appear in the default toxicity data table. The following subsections have titles identical to the column titles in the data tables. Part of the text in this chapter is cited from Traas (2001).

2.2.4.1 Species/process/enzymatic activity

See section 2.2.3.1 for guidance on reporting data on species. Enzymatic reactions are listed as follows:

Enzymatic activity
Amylase
Dehydrogenase
Phosphatase
Urease
etc.

Microbial processes are listed as follows:

Microbial processes
Ammonification
Nitrification
Respiration
etc.

2.2.4.2 Species properties

See section 2.2.3.2.

2.2.4.3 Soil/sediment type

In this column, list the soil or sediment type: e.g. sandy loam, clay for soils; for sediments: fine sandy or organic rich, muddy. If percentages of clay, sand and silt are given, the soil type can be derived using the soil texture triangle of the American Soil Classification System (see Appendix 3: Soil classification).

2.2.4.4 Analysed

See section 2.2.3.3.

2.2.4.5 Test compound

See section 2.2.3.5.

2.2.4.6 Purity

See section 2.2.3.6.

2.2.4.7 pH

Report the pH or the range of pH values, of the test soil or sediment in this column.

2.2.4.8 Organic matter (om)
Unit: %
In this column the weight percentage of organic matter in the soil or sediment is reported. When in a study the percentage organic carbon is given, recalculation to percentage organic matter (om) is necessary according to Eq. 2:

$$\%\ om = 1.7 \times \%\ oc \qquad (2)$$

This is the general conversion between organic matter and organic carbon used throughout the whole process of deriving risk limits. The value of 1.7 is derived from the TGD (standard soil in the TGD contains 2% o.c. or 3.4% o.m.).

2.2.4.9 Clay
Unit: %
In this column the weight percentage of clay in the soil or sediment is reported. The % clay (lutum) is used to convert test results for metals to standard soil and sediment. Further, this gives valuable information on the type of soil or sediment used.

2.2.4.10 Temperature
See section 2.2.3.9.

2.2.4.11 Exposure time
See section 2.2.3.12.

2.2.4.12 Criterion
Extensive information on the criteria is given in section 2.2.3.13. In addition, in terrestrial ecotoxicology, microbial processes are often studied. In studies submitted in the pesticide registration framework, two concentrations are usually tested in such studies: one equal to and another one 10 times the application rate in the field. If a test results in two effect concentrations, an EC10 is calculated using a logistic dose-response model (e.g. with GraphPad Prism (GraphPad Software, 2003), or a calculation in MS Excel). The EC10 value obtained is considered to be the NOEC. Prerequisite is that these effect concentrations (EC) differ by more than 15% and are lower than the EC70. If the difference between the two EC-values is less than 15%, their average value is considered to represent one EC-value. In order to be used in ERL derivation, the average EC-value should be below 20% effect. ECx data are treated in the same way as ECx data for aquatic species (section 2.2.3.13). A similar approach can be followed for sediment if studies on microbial processes in sediment are available.

2.2.4.13 Test endpoint
See section 2.2.3.14.

2.2.4.14 Result test soil/sediment
Unit: $mg.kg^{-1}$, $\mu g.kg^{-1}$
The unit in which the results of toxicity tests are expressed is optional. For reasons of comparison and to avoid errors, the same unit is used throughout all terrestrial and benthic toxicity data tables. This column shows the result as obtained in the experiment, expressed in weight units per kg dry weight of the test soil (i.e. *not* recalculated to standard soil or sediment). For further guidance, see section 2.2.3.15.

2.2.4.15 Result standard soil/sediment

Unit: $mg.kg^{-1}$, $\mu g.kg^{-1}$

The unit in which the results of toxicity tests are expressed is optional. For reasons of comparison and to avoid errors, the same unit is used throughout all terrestrial and benthic toxicity data tables. This column shows the result recalculated into weight units per kg of standard soil or sediment (dry weight).

The bioavailability of compounds in soil and sediment is influenced by properties like organic matter content, clay content, pH, moisture content etc. This hampers direct comparison of toxicity results obtained for the same substance in different soils or sediments. In order to make results from toxicity tests conducted in different soils or sediments more comparable, results should be normalised using relationships that describe the bioavailability of the compound in soil and sediment. Results are converted to a Dutch standard soil or sediment, which are defined as having an organic matter content of 10% (w/w, or 5.88% organic carbon; see section 2.2.4.8) and a lutum (clay) content of 25%.

Organic compounds

For non-ionic organic compounds, it is assumed that bioavailability is determined by organic matter content only. In the TGD, it is advised to recalculate data from terrestrial toxicity experiments to the standard soil from the TGD. Within the framework of INS, this recalculation of results from individual tests (LC50s, EC50s, EC10s, NOECs) to Dutch standard soil and sediment is performed according to Eq. 3, with the organic matter content of Dutch standard soil and sediment:

$$TEST\ RESULT_{\text{Dutch standard soil/sediment}} = TEST\ RESULT_{\text{experimental soil/sediment}} \times \frac{F_{\text{om Dutch standard soil/sediment}}}{F_{\text{om experimental soil/sediment}}} \qquad (3)$$

N.B. The TGD states the following with respect to normalisation to standard soil:

> 'It should be noted that this recommended normalisation is only appropriate when it can be assumed that the binding behaviour of a non-ionic organic substance in question is predominantly driven by its log K_{ow}, and that organisms are exposed predominantly *via* pore water.'

However, no guidance is given for those compounds to which the above statement does not apply, e.g. ionisable organic compounds.

Guidance on recalculation to standard sediment is not reported in the TGD, nor in the FHI document. However, in the software program EUSES (European Union System for the Evaluation of Substances; European Commission, 2004a), this routine is built in for benthic toxicity studies using the same methodology as described above using sediment characteristics. (NB this is different from EqP calculations, where suspended matter characteristics are used to derive sediment PNECs, see section 3.7.2.) For INS purposes, we propose to follow the same methodology as described here for soil and as interpreted in EUSES (using Dutch standard sediment characteristics).

Metals

The main text of the TGD states that 'data should be normalised using relationships that describe the bioavailability of chemicals in soils', but a method for the normalisation of toxicity data of metals for terrestrial and benthic organisms is not presented. However, in Appendix VIII of the TGD [footnote 9, p. 302], the methodology that has been followed in the Netherlands is reported. In the section on the effect assessment of the metals [page 309], the TGD states that this approach should be followed. This method makes use of so-called reference lines. In order to use these reference lines, both the organic matter and lutum content of the test soil and a standard soil need to

be known[13]. Using this method, it is possible to normalise toxicity data of metals to Dutch standard soil and Dutch standard sediment, both containing 10% organic matter and 25% lutum. The method can be found in section 4.4.2.1 of RIVM report 601501012 (Traas, 2001).

There are arguments against the normalisation of metal toxicity data.
1. The reference lines were developed as soil type correction for background concentrations rather than as a bioavailability-correction (Sijm *et al.*, 2002). In this document, Sijm *et al*. reported on a Dutch national workshop on bioavailability and its place in environmental policy (September 2001). It was concluded that improved bioavailability relationships should be developed for ERL derivation in the near future. At present, no improved relationships have been developed.
2. In four current drafts of EU risk assessment reports (EU-RARs, antimony, zinc, cadmium and chromate) normalisation of toxicity data to standard soil is not applied. This indicates that, following EU guidance, normalisation of soil toxicity data for metals is apparently not the preferential route. However, in other draft EU-RARs some more advanced methods for normalisation have been used (e.g. draft RAR on copper and nickel compounds).
3. In order to perform normalisation using the reference lines, the lutum or clay content of the soil used in the toxicity experiment should be reported. Since this is not the case for all soil toxicity studies, the number of available toxicity data that can be used for risk limit derivation would decrease. This would seriously affect the reliability of the risk limit.

In the three numbered sections above, soil can be read as synonym to sediment.

It is proposed, in general, not to normalise toxicity data for metals for the reasons mentioned above, if no improved bioavailability corrections are available in comparison with the reference lines. For ERL derivation, all reliable toxicity results with metals to soil or to benthic organisms are grouped in the appropriate data table without normalisation.

2.2.4.16 Validity
This column contains a number (1, 2, 3 or 4), indicating the quality of the study summarised. Section 2.2.2.1 describes the background of the quality scoring system.

2.2.4.17 Notes
See section 2.2.3.17.

2.2.4.18 Reference
See section 2.2.3.18.

2.2.5 Bird and mammal toxicity data tables
When secondary poisoning is assessed, results from toxicity studies with birds and mammals are tabulated in separate tables. Data on bioconcentration and biomagnification should be collected as well. For information on the collection of these parameters, see section 2.3 below. According to the TGD and FHI, data from single dosing are not taken into account for the assessment of secondary poisoning. An expert on human toxicology should be consulted when interpretation of toxicity tests with mammals is complex.

2.2.5.1 Species
See section 2.2.3.1

[13] Since the EU standard soil has no standard lutum content, normalisation of metal toxicity data to the EU standard soil using reference lines is not possible.

2.2.5.2 Species properties
See section 2.2.3.2

2.2.5.3 Product or substance
Toxicity studies on birds or mammals may also be carried out with formulations or products rather than individual substances. Report the name of the substance, product of formulation that has been used in this column.

2.2.5.4 Purity or a.i. content
In the case that a product (or formulation) is tested, report the content of active ingredient (a.i.) present in the product, expressed in %. If the purity of the active ingredient (used in formulation) is also known, report this in a footnote.
If a single substance has been applied in the test, report the purity of the tested compound in this column.

2.2.5.5 Application route
Relevant are those toxicity tests in which the animals are dosed orally. This might be achieved via a direct method (intubation, gavage) or by dosing via the food or water.
A short list of application routes is given below:

intubation
gavage
capsule
diet
water
feeding solution

2.2.5.6 Vehicle
A carrier used to dose the test substance to the test animals is reported here.

2.2.5.7 Test duration
The value in this column reports the total duration of the test. The abbreviations listed in Table 9 can be used. This column should also be filled in when the test duration is equal to the exposure duration. The test duration might be longer than the exposure time, which is reported in the next column (Exposure time). For example in the acute avian dietary toxicity test, in which the exposure lasts 5 days, but the minimal recommended test duration is 8 days.

2.2.5.8 Exposure time
The duration of exposure to the toxicant in the toxicity experiment is expressed in this column. The abbreviations listed in Table 9 can be used.

2.2.5.9 Criterion
Short term toxicity tests will either yield an LC50 ($mg \cdot kg_{food}^{-1}$) or an LD50 ($mg \cdot kg_{bw}^{-1} \cdot d^{-1}$ in the case of repetitive dosing). Long-term toxicity tests will generally result in a NOEC (no observed effect concentration in diet; $mg \cdot kg_{food}^{-1}$), or a NOEL (no observed effect level in a dosing study; $mg.kg_{bw}^{-1}.d^{-1}$). Results from long-term toxicity tests may also be reported as a NOAEL, which is the no observed adverse effect level. However, the effects generally observed for the derivation of the NOEC/NOEL are adverse to the organisms.

2.2.5.10 Test endpoint
The toxicological parameter for which the test result is obtained is tabulated here. Screening for clinical parameters at haematological, histopathological or biochemical level is common in these types of tests. The list below shows only some of the relevant endpoints:

body weight
egg production
eggshell thickness
hatchability
hatchling survival
histopathological findings
mortality
reproduction
viability (percentage of viable embryos per total number of eggs)

2.2.5.11 Value from repetitive oral dosing studies
Unit: $mg.kg_{bw}^{-1}.d^{-1}$.
See also section 2.2.3.15 for data handling.
From short term toxicity experiments with repetitive dosing on consecutive days (5 d LD50 for birds) and long-term oral dosing studies, a value expressed in $mg.kg_{bw}^{-1}.d^{-1}$ is obtained. The results from such studies (*viz.* LD50 and NO(A)EL) are reported in this column.

2.2.5.12 Value from diet studies
Unit: $mg.kg_{food}^{-1}$.
See also section 2.2.3.15 for data handling.
The results of toxicity tests in which the substance of interest is administered via the food are expressed in $mg.kg_{food}^{-1}$. The results of dietary studies (*viz*. LC50 or NOEC values) are reported in this column.

2.2.5.13 Validity
This column contains a number (1, 2, 3 or 4), indicating the quality of the study summarised. Section 2.2.2.1 describes the background of the quality scoring system.

2.2.5.14 Notes
See section 2.2.3.17.

2.2.5.15 Reference
See section 2.2.3.18.

2.2.6 Data selection
2.2.6.1 Aquatic compartment
One value per species is selected for use in the risk assessment. The individual tabulated toxicity data are aggregated to a new table with selected toxicity data according to the following guidance (Guidance TGD, FHI guidance cites the TGD on these topics[14]):

1. Evaluate the full data table on toxicity and identify particularly sensitive species and/or endpoints that may be lost upon averaging data to single values.

[14] In the FHI document this guidance is given in detail only in the section on statistical extrapolation. However, in a footnote to the general notes on the evaluation and selection of ecotoxicological data, this guidance is shortly summarised.

2. Demographic parameters and data from biomarkers may be used as endpoints if they are relevant in terms of population dynamics.
3. Investigate multiple values for the same endpoint on a case by case basis and look for the cause of differences between results. Although not mentioned in the guidance of the TGD, it is advised to address the relevant differences in the report section on the derivation of the MPC as well.
4. In the case that valid data show high variation, grouping of data or combining values is considered, e.g. by pH ranges.
5. If for a test species, an effect of test conditions is expected to be the cause of variation in toxicity values (hardness of test water, life stage of the test animal, etc.), averaging of data per species should not be performed.
6. Selection of data used for ERL derivation should then first be based on the likelihood of test conditions (pH, hardness, etc.) to occur in the field (e.g. in the Netherlands).
7. If the variation in test results of different life stages of a test animal is such that averaging data would cause significant underprotection of sensitive life stages, only the data for the most sensitive life stage should be selected. This aspect is not explicitly mentioned in the TGD, but in the evaluation of the data quality for the SSD method, it is stressed that it is important that sensitive life stages are covered.
8. Calculate the geometric mean of multiple comparable toxicity values for the same species and the same endpoint[15].
9. If multiple toxicity values or geometric means for different endpoints are available for one species, the endpoint for which the lowest value is obtained is selected. This step is not fully elaborated in the guidance of the TGD. When, after primary selection, multiple valid toxicity data for one species are left that can not be averaged, the *lowest* value is selected.

> Example. There are values (of NOECs or EC10 values) for three different endpoints, derived from several chronic studies with *Daphnia magna.* The geometric mean of NOECs for reproduction is 0.49 $mg.L^{-1}$, the geometric mean of NOECs for mortality = 3.1 $mg.L^{-1}$ and there is a single EC10 value for growth of 0.67 $mg.L^{-1}$. The geometric mean value of 0.49 $mg.L^{-1}$ for reproduction is selected for use in ERL derivation.

10. If it can be inferred that the chemical form of the test compound (congeners, stereoisomers, different metal salts or metal valence states, etc.) is the cause of variation in toxicity values for a test species, averaging of data per species should not be performed. In these cases, the *lowest* toxicity value is selected. In such a case it can be considered whether separate ERLs should be derived for each form of the test compound.
11. Limitations of toxicity data should be explained, for example, when toxicity results are not valid at low pH. Explanation for these types of limitations should be reported in the section where the ERLs are derived.

[15] TGD contains an omission here. Calculating the geometric mean of acute toxicity data when using preliminary effect assessment (applying assessment factors) is explicitly mentioned [TGD, section 3.3.1.1, p. 100] for those cases where more than one value is available for the same species and the same endpoint. However, this procedure is not mentioned for NOECs or EC10 values from chronic data. It is, however, mentioned to calculate geometric means from NOEC or EC10 from chronic data in the section on refined effect assessment [TGD, section 3.3.1.2, page 104]. In our opinion this 'averaging' procedure should also apply to chronic data that are used in preliminary effect assessment.

2.2.6.2 Terrestrial and sediment compartments

The TGD presents the guidance shown above for data treatment of aquatic toxicity studies. For soil and sediment this guidance is not explicit. However, for soil, the TGD recommends normalising the results of terrestrial toxicity studies with organic compounds to standard soil (see section 2.2.4.15) in order to make results from studies with different types of soil comparable. For this reason, the guidance given above for water is considered to be valid for test results of organic substances in soil and sediment as well, but only after normalisation to standard soil or sediment.

Although for some metals a normalisation to a standard soil can be performed, it is recommended not to normalise the results of terrestrial toxicity experiments with metals to standard soil (section 2.2.4.15), because even after normalisation, soil properties can influence the outcome of the experiment, i.e. they may also determine the height of the concentration exerting a certain effect (L(E)C50 or NOEC). For this reason, individual toxicity results for one species or process with the same endpoint are not averaged, but the lowest value is selected. However, in the case that all test conditions are the same, there are two possibilities:

- when more than one toxicity result is available for the same species (or process or enzyme reaction) in the same soil, for the same valence state of the element and for the same endpoint, the geometric mean of the results should be calculated.
- when more than one toxicity result is available for the same species (or process or enzyme reaction) in the same soil, for the same valence state of the element and for different endpoints, the lowest of these values should be selected.

2.2.7 Data treatment

2.2.7.1 Combining freshwater and marine data sets for ERL derivation

Both FHI and TGD [FHI, section 4.3.2.2, p. 18; TGD, section 4.3.1.2, p. 147-148] give highly comparable guidance on the issue of combining freshwater and marine aquatic toxicity datasets. The FHI cites the TGD for this subject. A quotation from FHI makes the guidance quite clear.

> **FHI, section 4.3.2.2. p. 18:**
> 'In order to derive environmental quality standards for transitional, coastal and territorial waters combined toxicity data sets of marine and freshwater species are normally used as toxicity data because current marine risk assessment practice suggests a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota [TGD] (i.e. the same data sets can be used interchangeably for freshwater and saltwater effects assessment and QS setting). Where this appears not justified based on the available evidence, EQS for inland surface waters and transitional, coastal and territorial waters must be derived on the basis of distinct data sets for freshwater and marine organisms.'

Guidance for INS is as follows:
In practice, toxicity data for freshwater organisms and marine organisms are combined *before* ERL derivation for the aquatic compartments. If there are doubts as to whether organisms from both environments show similar sensitivity, differences are tested in the following way:

1. All freshwater data that are going to be used for risk limit derivation are collected (note: this data set contains one toxicity value per species, see section 2.2.6.1). Next, the $\log_{10}$ value of each of these toxicity values is calculated.

2. All marine data that are going to be used for risk limit derivation are collected (note: this data set contains one toxicity value per species, see section 2.2.6.1). Next, the $\log_{10}$ value of each of these toxicity values is calculated.
3. It is investigated whether the two log-transformed data sets have equal or unequal variances using an *F*-test. Perform the test at a significance level (α) of 0.05.
4. A two tailed *t*-test, with or without correction for unequal variances as determined in point 3, is performed to test for differences between the data sets. Perform the test at a significance level (α) of 0.05.
5. When using a statistical test, be aware of some confounders. For example: (i) a specific group of organisms might be more sensitive than other organisms; (ii) overrepresentation of results from one study or species from a specific taxonomic group in one of the two data sets might cause biased results. Results of a *t*-test become increasingly meaningful with increasing sample size.

Exceptions: Plant protection products and metals
Two exceptions to the above-mentioned principle are made in the TGD and FHI documents. The TGD [section 4.3.1.2, page 148] states that within trophic levels differences larger than a factor of 10 were shown for several metals and pesticides, indicating that for these substances freshwater and saltwater data should not be combined.
For plant protection products (PPP), FHI [section 4.3.2.2. p. 18 and section 4.3.4.4. p. 31] refers to the TGD, stating that freshwater data shall normally not be used in place of saltwater data[16].
According to the FHI guidance the derivation of ERLs for these compounds for transitional, coastal and territorial waters is *not* possible if:

(i) there are no effect data for marine organisms available, or
(ii) if it is not possible to determine otherwise with high probability that marine organisms are not more sensitive than freshwater biota (consideration of the mode of action may be helpful in this assessment).

The or-statement in the FHI guidance is probably a mistake. To our opinion the guidance should be interpreted as such: for plant protection products it is possible to derive environmental quality standards provided that effect data for marine organisms are available, or that it is possible to determine with high probability that marine organisms might not be more sensitive than freshwater biota.

Additional guidance
FHI guidance at this point is unclear. Although it is not stated what the effect data for marine organisms should comprise, it can be argued that, similar to the freshwater compartment, the minimum set for the marine environment should be algae, crustaceans and fish. However, it is indicated that if other types of information are available, showing whether or not saltwater organisms are more sensitive than freshwater organisms, ERLs might be derived. This implies that this derivation should be done on basis of the available freshwater data. Besides this, also on the basis of marine toxicity data, there might be strong indications that saltwater organisms are not more sensitive than freshwater organisms. However, to prove with high probability that data are different, a *t*-test can be carried out, in which the significance level is set at 0.05. Or, if a higher probability is needed, a lower significance level of 0.01 is set, for example, but the negative formulation to the opposite (as formulated in the FHI guidance) can not be statistically tested. Therefore, the same two-sided *t*-test on the available data could be used for PPP, with the exception that the test is used more strictly and that –where there is doubt – both data sets are considered as

[16] INS addition: the reverse is also true here, i.e. do not use data for saltwater organisms for a freshwater ERL derivation.

having different sensitivities. Information that might facilitate the forming of an opinion on this matter are 'read across' with structurally closely related substances and knowledge on the mode of action, the latter also being mentioned in the FHI guidance.

The FHI document gives some additional specific guidance for metals. Toxicity data sets and BCF data sets for metals should be compared for differences in sensitivities at the level of *taxonomic groups* [FHI, section 4.4.3, p. 42]. When a difference in sensitivity is observed between freshwater and marine species belonging to the same taxonomic group, marine and freshwater data sets should not be combined. MPCs for freshwater and marine water should then be derived on the basis of separate data sets.

2.2.7.2 Conversion of data on birds and mammals

For each of the selected avian or mammalian toxicity studies, the test result is expressed as a $NOEC_{oral}$ in $mg.kg_{food}^{-1}$. No observed adverse effect concentrations (NO(A)ELs, expressed on a basis of $mg.kg_{bw}^{-1}.d^{-1}$), are converted to $NOECs_{oral}$ (in $mg.kg_{food}^{-1}$) using the following equations, with the conversion factors from Table 11 or a suitable factor for the daily food intake for any other species:

$$NOEC_{\text{bird}} = NOAEL_{\text{bird}} \cdot CONV_{\text{bird}} \quad (4)$$

$$NOEC_{\text{mammal,food\_chr}} = NOAEL_{\text{mammal,oral\_chr}} \cdot CONV_{\text{mammal}} \quad (5)$$

Table 11. Conversion factors from NOAEL to NOEC for several species.

Species	Common name	Conversion factor ($bw.dfi^{-1}$)
Canis domesticus	Dog	40
Macaca sp.	Macaque species(monkey)	20
Microtus spp.	Vole species	8.3
Mus musculus	House mouse	8.3
Oryctolagus cuniculus	European rabbit	33.3
Rattus norvegicus (>6 weeks)	Brown rat	20
Rattus norvegicus (≤ 6 weeks)	Brown rat	10
Gallus domesticus	Chicken	8

bw = body weight (g); dfi = daily food intake ($g.d^{-1}$).

2.3 Bioconcentration and biomagnification data

2.3.1 Data collection

The literature should be searched for BCF and BMF studies if the log K_{ow} value of the substance is equal to or larger than 3, or if there is any other indication of a bioaccumulation potential of the substance. Useful data sources for BCF values are the physical-chemical properties and environmental fate handbook (Mackay *et al.*, 2006) and ECOTOX (U.S. EPA, 2007a), of which the latter can be accessed via the e-toxBase of RIVM as well. If valid experimental data show that BCF ≥ 100, this BCF value triggers the derivation -following FHI guidance (section 3.1.1)- of two aquatic ERLs,. The first is for adverse human health effects due to the consumption of fishery products. The second is for the secondary poisoning of predators through the aquatic compartment. When BMF studies are found showing that there is potential for biomagnification (BMF > 1), this also triggers incorporation of both routes in the ERL derivation. Results from the studies are tabulated in separate BCF and BMF tables.

2.3.2 Data evaluation and data tables

In principle, the evaluation of bioaccumulation data follows the evaluation for toxicity to a large extent. All retrieved literature is read and evaluated with respect to its usefulness and reliability. The most relevant BCF studies are those performed with fish. BCF studies performed with molluscs are important for secondary poisoning as well. BCF data for other species should be carefully checked because they are prone to experimental errors. The accumulation may not reflect uptake but adsorption to the outside of the organism. For this reason, BCF values for algae should be regarded as unreliable. A reliable BCF study should be similar in experimental set-up to the updated OECD guideline 305 (OECD, 1996). At least the concentration of the (parent) compound in the aqueous phase, and in fish, has to be measured at several time points. No guidance is available for BMF studies. BMF data will be mostly derived from field studies. Apart from the analysis, for a reliable BMF value it is necessary to know that the prey and predator species originate from the same area and from the same period in time. After evaluating a study, the results of the study are summarised by entering it into the appropriate data table. The guidance in section 2.3.3 is followed for this purpose.

2.3.3 Bioconcentration data tables

The following sections (2.3.3.1 to 2.3.3.17) discuss the parameters that are to be reported in the BCF data tables. The aim is to fill the table as completely as possible. The parameters are treated in the same order as they appear in the default BCF data table The following subsections have titles identical to the column titles in the data tables.

Note. In the following sections, fish are mentioned as the test organism most frequently encountered in BCF studies. However, BCF studies with mussels may also be retrieved. These data are relevant, as the food chain water → mussel (→ fish) → mussel/fish eating bird or mammal is also considered of importance (see section 3.1.4). The TGD offers the opportunity to incorporate this route, since an $MPC_{oral,\ predator}$ ($PEC_{oral,\ predator}$ in the TGD, p.126) 'could also be calculated for other relevant species that are part of the food of the predators'. The following sections each describe the content of the columns that make up the BCF data table.

2.3.3.1 Species

See 2.2.3.1.

2.3.3.2 Species properties

See 2.2.3.2.

2.3.3.3 Test substance

Clearly report what compound is used. If a radiolabelled compound is used, it should be reported in this column of the BCF data table For organic compounds that have one or more isomers, the specific isomer (or mixture of isomers) used in the test is reported, e.g. diastereomers, *cis*/*trans* conformation, *o*, *m*, *p* substitution, formulations, etc.

2.3.3.4 Substance purity

See 2.2.3.6.

2.3.3.5 Analysed

Similar to the toxicity data tables, a column in the BCF data table is included that gives information on the analysis of both the aqueous phase and biological material. However, as the determination of the water and biota concentration is a prerequisite of any good BCF study, this column should give

information on how the concentration is determined, not on whether the concentration is determined. Examples of such analyses are GC-FID or GC-MS (gas chromatography coupled to a flame ionisation detector or a mass spectrometer), and HPLC-UV (high-performance liquid chromatography). Especially in the case that a radiotracer is used, the analysis used is important. If LSC (liquid scintillation counting) is used, this means that the total radioactivity, including the parent compound and metabolites, is analysed. HPLC used in combination with radiodetection is aimed at analysis of only the parent compound.

2.3.3.6 Test type
See 2.3.3.6.

2.3.3.7 Test water
See 2.2.3.7.

2.3.3.8 pH
See 2.2.3.8.

2.3.3.9 Hardness/Salinity
See 2.2.3.10 and 2.2.3.11.

2.3.3.10 Temperature
See 2.2.3.9.

2.3.3.11 Exposure time
In this column, the times of the uptake phase and, if carried out, the depuration phase are listed. If both phases are determined, the exposure time and depuration time are listed as two separate time spans: e.g. 14+14 d.

2.3.3.12 Exposure concentration
The concentration at which the BCF study is performed is given in this column of the BCF table . This value is important because guidelines require that the concentration meets some conditions. For example, according to the OECD guideline 305 (OECD, 1996), the highest aqueous concentration should be about one hundredth of the acute LC50 or the acute LC50 divided by an appropriate acute-to-chronic ratio, while the lowest concentration should preferably be a factor of ten below the highest concentration, but at least ten times above the limit of detection in the aqueous phase.

2.3.3.13 BCF
Unit: $L.kg^{-1}$.
Here, the value of the BCF is denoted. The basis for the BCF value is the ratio of the concentration in wet weight (ww) of the organism, mostly fish, divided by the water concentration. The unit of the BCF is $L.kg_{ww}^{-1}$; if the BCF is normalised to dry weight or lipid weight, this should be explicitly indicated with a note describing the origin of the value.

BCF values used for triggering and calculating the routes of secondary poisoning and human consumption of fishery products should be whole body BCFs, expressed in $L.kg^{-1}$. It is realised that this allows for variation since these BCFs are not normalised to lipid or fat content, which dominates accumulation. ERL derivation is purely dependent on the available studies. In most older BCF studies, fat content is often not reported. Because, there is no possibility to request studies for the purpose of ERL derivation, requirements with respect to normalisation are not applied. This is

preferred above excluding the data, which would possibly result in bioaccumulative substances not being triggered.

2.3.3.14 BCF type

In this column in the table, it is reported what part of the organism the BCF has been determined for. Possibilities are (e.g.): whole fish ww, whole fish dw, edible parts, non-edible parts viscera, etc.

2.3.3.15 Method

The method that is used to calculate the BCF value is reported in this column. Basically, the method to calculate the BCF can be based on equilibrium concentrations or on kinetics including the uptake and depuration rate constants (k_1 and k_2). With equilibrium concentrations (noted as equilibrium), the BCF is determined as the quotient of the concentrations in organisms, mostly fish, and water at equilibrium. When the kinetic constants (k_1/k_2) are used to calculate the BCF, the BCF is calculated as the quotient of uptake rate (k_1) and depuration rate (k_2), mostly determined independently during an uptake and a depuration phase (k_1, k_2 independent). However, in some studies, k_2 is first determined from the depuration phase and k_1 estimated from the data of the uptake phase, with this value of k_2 implied to take the non-linearity of the uptake into account (k_1 implied by fitted k_2). A further possibility is that k_1 and k_2 are fitted simultaneously by a non-linear regression model.
If the method can not be shortly described, a reference to a note below the table can be entered here. The method is described in more detail in the note.

2.3.3.16 Notes

Additional notes are recorded here by a number. Notes are listed below the table. The notes may include information on the analysis, a deviating basis of the BCF value (dry weight or lipid weight) or the method used to determine the BCF.

2.3.3.17 Reference

See 2.2.4.18.

2.3.4 Data selection

2.3.4.1 BCF - experimental data

Aquatic compartment

From the valid BCF studies summarised in the BCF data table (section 2.3.3) calculate the geometric mean values per species. Of these values per species, the most reliable or the geometric mean of several BCFs that are considered equally reliable is selected. This selected BCF value is tabulated as described in section 3.1.1 (Table 15).

Metals

FHI guidance [section 4.4.4] gives the following guidance referring to the selection of BCF values for metals:

1. 'BCF values (for metals) determined in studies conducted at extremely low or high metal concentrations should not be used for derivation of quality standards'. In the FHI document, extremely low is defined as 'lower than in the upper range of background levels', while 'high' is not defined.
2. The BCFs used for the derivation of the risk limits should be calculated from:
   (i) 'species specific geometric means from BCF studies with environmentally relevant metal concentrations in the test media';
   (ii) 'field determined BCFs'.

ad (i). Although high metal concentrations are not defined as such in the TGD and FHI, it should be evident that similar to determining the BCF for organic substances (e.g. with OECD guideline 305 OECD, 1996), the concentration should be well below toxicity levels.

Terrestrial compartment
A bioaccumulation test with earthworms can be performed according to a draft OECD guideline (UBA, 2002). In this test worms are exposed for at least 21 days to non-toxic concentrations of the substance. Then, for at least another 21 days they are kept in clean soil to study the elimination. Concentrations are monitored at regular time intervals. All tests that use this or a similar test design can be considered to be a valid bioaccumulation study for the terrestrial compartment. For organic chemicals the accumulation factor to be used in the derivation of risk limits should be normalised from the organic carbon content of the soil in the study to the organic carbon content of Dutch standard soil in the same way as for toxicity studies (see section 2.2.4.15).

2.3.4.2 BCF - calculation method

Aquatic compartment
When a BCF can not be derived on the basis of experimental data, check the log K_{ow} value of the compound of interest. BCF values are only needed in further ERL derivation when log $K_{ow} \geq 3$. When log $K_{ow} \geq 3$, calculate a BCF according to the method cited from the TGD [section 3.8.3.2, p. 126], which is described in the following section:

BCF calculation according to TGD guidance:
'If measured BCF values are not available, the BCF for fish can be predicted from the relationship between K_{ow} and BCF. Various methods are available to calculate K_{ow}. Often a large variation is found in the K_{ow} values of a chemical by using different methods. Therefore the K_{ow} value must have been evaluated by an expert (see also Chapter 4 of TGD part III (European Commission (Joint Research Centre), 2003b) on the use of QSARs). For substances with a log K_{ow} of 2 – 6, the following linear relationship, as developed by Veith *et al*. (1979), can be used:

$$\log BCF_{\text{fish}} = 0.85 \times \log K_{ow} - 0.70 \qquad (6)$$

For substances with a log K_{ow} higher than 6, a parabolic equation can be used:

$$\log BCF_{\text{fish}} = -0.20 \times \log K_{ow}^{\,2} + 2.74 \times \log K_{ow} - 4.72 \qquad (7)$$

It should be noted that due to experimental difficulties in determining BCF values for such substances this mathematical relationship has a higher degree of uncertainty than the linear one. Both relationships apply to compounds with a molecular weight of less than 700. For a discussion on both relationships see Chapter 4 of TGD part III (European Commission (Joint Research Centre), 2003b).

Terrestrial compartment
When experimental bioconcentration data on earthworms are not available, estimate the BCF using Eq. 8. This equation can be used to estimate $BCF_{earthworm}$ for organic compounds.

$$BCF_{earthworm} = 0.84 + \frac{0.012 \cdot K_{ow}}{RHO_{earthworm}} \qquad (8)$$

This equation relates to pore water. The bioaccumulation from soil can be calculated from this value and the soil-water partition coefficient.

2.3.4.3 BMF – experimental data

Experimental BMF values generally originate from field studies. From the valid BMF studies summarised in a BMF data table, the geometric mean value is calculated. This final BMF value is tabulated as described in section 3.1.1 (Table 15).

2.3.4.4 BMF - calculation method

When a BMF can not be derived on the basis of experimental data, check the log K_{ow} value of the compound of interest. BMF values are only needed in further ERL derivation when log $K_{ow} \geq 3$. If log $K_{ow} \geq 3$ and experimental data on BMF are not available, default BMF values will be selected, depending on the log K_{ow} of the compound of interest. At present, calculation methods to derive BMF values are not in use. Both the FHI document and the TGD give the same default values for the biomagnification factors, as reported in Table 12 below. In this table, BMF_1 is a value for the biomagnification in the prey of predators for the freshwater environment. For the marine environment, an additional biomagnification step is included, which is reflected in the BMF_2 value. This BMF_2 is a value for biomagnification in the prey of top predators.

The most relevant values for BMF_1 are those for biomagnification from small to larger fish (either fresh or marine water). These larger fish then serve as food for predators such as otters and herons, and seals in the marine environment. Data for biomagnification from other small species such as crustaceans to fish might be useful as well, but care must be taken that in the further assessment of secondary poisoning, BCF and BMF values are in accordance with each other (see section 3.1.4). For comparison, the default values from Table 12 can be used. Another group of prey that might be relevant to the route of secondary poisoning are mussels. If mussels are directly consumed by birds or mammals and a BCF value for mussels is available, a biomagnification step would be absent. However, there are also several common fish species that feed on mussels. In such a case BMF data on accumulation from mussels to fish would be relevant (see section 3.1.4).

For the marine environment another biomagnification step is considered by introducing the BMF_2 value. This step refers to the biomagnification from fish to small mammals and birds. For the marine environment, a good example is the biomagnification from fish to seals. The latter species then serve as prey for top predators such as polar bears and killer whales. However, besides data for the marine environment, other data for biomagnification from fish to fish-eating birds and mammals should be considered as well.

Table 12. Default BMF-values for organic substances.

log K_{ow} of substance	BCF (fish)	BMF_1	BMF_2
< 4.5	< 2000	1	1
4.5 - < 5	2000-5000	2	2
5 – 8	> 5000	10	10
> 8 – 9	2000 – 5000	3	3
> 9	< 2000	1	1

Column 2 of Table 12 also shows (ranges of) BCF values. These values are, however, not used, which is explained in the following. If one or more experimental BCF data are available, the BCF values from the tables are not needed. If there is no experimental BCF value, the numbers from Table 12 can not be regarded as guidance, because they represent ranges instead of single values. In such a case, it is better to estimate the BCF from the log K_{ow}, according to the QSARs proposed in

the TGD. This procedure is described in section 2.3.4.2. The results are largely in accordance with the ranges presented in Table 12.

2.4 Human toxicological data

2.4.1 Threshold limits

A human toxicological threshold value is needed at several places in ERL derivation:
- in the derivation of the $MPC_{hh\ food,\ water}$ (section 3.1.5, for consumption of fishery products)
- in the derivation of the $MPC_{dw,\ water}$ (section 3.1.6, for drinking water)
- in the derivation of the $MPC_{human,\ comp}$ (section 3.3.6, for exposure via soil, via multiple routes).

The human toxicological threshold values that can be used are the ADI (acceptable daily intake) and TDI (Tolerable Daily Intake). The U.S. ATSDR uses the term MRL (minimum risk level) while the U.S. EPA uses the term RfD (reference dose). The basis for the human-toxicological threshold levels is in principle a NO(A)EL from a mammalian toxicity study, which is useful as well if established threshold levels are unavailable. However, the NOAEL is not a human toxicological threshold limit. In principle, the applied assessment factor is 100 (e.g. see FHI document, section 4.3.3, page 27). To derive a TDI or ADI from a NOAEL a human toxicologist should be consulted in any case.

With respect to human toxicological threshold values, the FHI main report (Lepper, 2002), p. 95 states the following:

> 'Effect data used in deriving quality standards referring to human health are, for instance, the relevant NOAEL, ADI, TDI values identified in the human health section of risk assessments according to Council Regulation (EEC) No. 793/93 or Council Directive 91/414/EEC. ADI or TDI values adopted by international bodies such as the World Health Organization may also be used. For effects for which a threshold level cannot be given, unit risk values corresponding to an additional risk of, e.g., cancer over the whole life of 10^{-6} (one additional cancer incident in 10^{6} persons taking up the substance concerned for 70 years) may be used, if available. Only data from reliable sources will be used.'

A list of organisations or frameworks that have published human toxicological threshold limits is presented in Table 13 (extracted from Hansler *et al*., 2006). In general, it is advised to take the most recent value and consult a human toxicologist on the final choice of the value. If a clear value is reported in a European Risk Assessment Report, or a value for $\mathbf{MPC_{human}}$ is derived in the Netherlands within INS framework, these values should preferably be used, provided that they are not outdated.

Table 13: Sources for the retrieval of human toxicological threshold limits.

Source name and publisher	Available at
HSDB (NLM / NIH)	http://toxnet.nlm.nih.gov/
ATSDR Toxicological Profiles (ATSDR)	http://www.atsdr.cdc.gov/mrls.html (MRLs) http://www.atsdr.cdc.gov/mrllist_12_05.pdf
CEPA Priority Substances Assessments (Environment- & Health-Canada)	http://www.cen-rce.org/eng/projects/cepa/
CICAD (IPCS)	http://www.inchem.org/pages/cicads.html
EHC (WHO/IPCS)	http://www.inchem.org/pages/ehc.html
ESIS (ECB)	http://ecb.jrc.it/esis/
HSG (WHO)	http://www.inchem.org/pages/hsg.html
IARC Monographs (WHO)	http://monographs.iarc.fr

Source name and publisher	Available at
ICSC (IPCS-EU)	http://www.inchem.org/pages/iarc.html http://www.inchem.org/pages/icsc.html
for pesticides, use:	http://www.inchem.org/documents/jmpr/jmpeval/jmpr2002.htm
IRIS (US-EPA)	http://www.epa.gov/iriswebp/iris
JECFA Monographs (WHO/FAO)	http://www.inchem.org/pages/jecfa.html
JMPR Monographs (WHO/FAO)	http://www.inchem.org/pages/jmpr.html
WHO/FAO (pesticides)	http://www.fao.org/docrep/W3727E/w3727e00.HTM
MPC_{human} values for the derivation of SRC_{human}	http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf
NTP (NIH-NIEHS)	http://ntp-server.niehs.nih.gov/
OEHHA Toxicity Criteria Database (Cal-EPA)	http://www.oehha.org/risk/chemicalDB/index.asp
SIDS (OECD-UNEP)	http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html
TERA (TERA)	http://www.tera.org/ITER.
DWQG (WHO)	http://www.who.int/water_sanitation_health/dwq/guidelines/en/
Umwelt-Online	http://www.umwelt-online.de/recht/gefstoff/g_stoffe/adi.htm

2.4.2 Data collection for $MPC_{human, soil}$ calculation

This section lists the parameters needed to calculate $MPC_{human, soil}$ values, as shown in Table 14. The parameters should be identical to those selected according to the methods and criteria described in the section 2.1.3. Section 3.3.6 describes the calculation method for the desired MPCs.

Table 14. Parameters required to calculate $MPC_{human, comp}$.

Parameter	Name/Description	Unit
M_w	molecular weight (only needed when a value for H is absent)	[g.mol^{-1}]
P_v	vapour pressure (only needed when a value for H is absent)	[Pa]
S_w	water solubility	[mg.L^{-1}]
H	Henry coefficient	[Pa.m^3.mol^{-1}]
K_{ow}	*n*-octanol water partition coefficient	[-]
K_{oc}	organic carbon normalised partition coefficient	[L.kg^{-1}]
MPC_{human}, TDI, ADI or similar	maximum permissible concentration for humans	[µg.kg$_{bw}^{-1}$.d^{-1}]

3. Derivation of MPC

3.1 Aquatic compartment

3.1.1 Trigger values

Prior to determining MPC values, the following information is collected and tabulated (see format of Table 15). This information is used to present the compound properties relevant for comparison to trigger values, as set down in the FHI document:

1. log $K_{p,\ susp\text{-}water}$;
2. BCF and/or BMF and/or log K_{ow};
3. Risk phrases (R phrases) that are applicable to the substance (classification and labelling);
4. If available, an 'A1 value' for the substance;
5. If available, a 'DW standard' for the substance.

Ad. 1. $K_{p,\ susp\text{-}water}$ is the distribution coefficient describing the partitioning of the compound between suspended particulate matter and water, expressed in $L.kg^{-1}$. Following FHI guidance, the value of this parameter triggers derivation of $MPC_{sediment}$: when $\log K_{p,\ susp\text{-}water} \geq 3$ for the compound of interest, $MPC_{sediment}$ should be derived. $K_{p,\ susp\text{-}water}$ is also needed in EqP calculations. For organic substances, this parameter is usually calculated from the K_{oc} (see section 2.1.3.3). For metals, this value is preferably derived from experimental data as collected according to section 2.1.2.6. The K_p for metals is calculated as the geometric mean of all available and valid K_p values for suspended matter or, alternatively, for sediment.

Ad. 2. See sections 2.1 and 2.3 for guidance on derivation of the log K_{ow}, and BCF and BMF data, respectively. If experimentally determined BCF and BMF values are not available, only log K_{ow} is tabulated.

Ad. 3. R phrases of the compound of interest can be retrieved from the internet at http://ecb.jrc.it/ by opening the information system ESIS, where the compound can be searched for e.g. by CAS registry no.

Ad. 4. A1 values are listed in Appendix 1 (this report); these are taken from Commission Directive 75/440/EEC (European Commission, 1975).
As defined in CD 75/440/EEC, A1 is a category of standard methods for the transformation of surface water into drinking water. A1 is defined as 'Simple physical treatment and disinfection, e.g. rapid filtration and disinfection'. An A1 value designates the maximum concentration of a substance at which it can still be removed when A1 treatment of surface water is applied.

Ad. 5. DW standards are listed in Appendix 2 (this report); these are taken from Commission Directive 98/83/EC (European Commission, 1998).
DW standard means 'drinking-water' standard, and is a concentration of a substance never to be exceeded in water intended for human consumption ('at the tap').

Table 15. Table format for collected properties for comparison to MPC triggers.

Parameter	Value	Unit	Derived at page nr.	Method (if applicable)
log $K_{p,\ susp\text{-}water}$		[-]		
BCF		[$L.kg^{-1}$]		
BMF		[-]		
Log K_{ow}		[-]		
R phrases	R XX, R XX			
A1 value	XXX / not available	[$mg.L^{-1}$]		
DW standard	XXX / not available	[$mg.L^{-1}$] or [$\mu g.L^{-1}$]		

For the above parameters and their values, Table 16 is checked to determine which quality standards should be derived, and Table 17 is checked to determine which route should be followed for the derivation of human health related limits [cited from FHI: tables 1a and 1b, p. 4].

Table 16. Environmental protection objectives and triggers to derive quality standards (cited from FHI).

Water (protection of the pelagic community)	**Sediments** (suspended particulate matter) (protection of the benthic community)	Substance concentration in **Biota** (prey; protection of predators against secondary poisoning)
No trigger value applies. EQS are derived for <u>all</u> priority substances. For hydrophobic / adsorbing substances the EQS referring to the concentration in water are additionally reported as concentration in suspended particulate matter (spm[17]) if this is meaningful. Trigger value: log $K_{p,\ susp\text{-}water} \geq 3$	EQS are derived for all substances with a log $K_{p,\ susp\text{-}water} \geq 3$ The $EQS_{sediment}$ refers to suspended particulate matter in order to protect the new sediment.	EQS are derived for organic substances and metals with experimental BCF $\geq$ 100 or BMF >1. If a reliable BCF is not available, the trigger is log Pow $\geq$ 3 (applies only to organic substances)[18]. In order to avoid routine monitoring of biota the concentrations in animal tissue are normally transformed to concentrations in water or suspended particulate matter, using appropriate model estimates / partition coefficients. However, if the partition coefficients are highly variable or uncertain, the setting of biota standards may be considered.

[17] Suspended matter (spm) is abbreviated by susp throughout this report.
[18] Pow is synonym to K_{ow}.

Table 17. Human-health related protection objectives and triggers to derive quality standards (cited from FHI).

Substance concentration in **Biota** (fishery products; protection of humans against adverse effects upon consumption of fishery products)	**Possibility to abstract drinking water from surface water**
An EQS is derived for substances: 1. being a known or suspected carcinogen (cat. I-III, R phrases R45 or R40) 2. being a known or suspected mutagen (cat. I-III, R phrases R46 or R40) 3. being a substance known or suspected to affect reproduction (cat. I-III, R phrases R60, R61, R62, R63 or R64) 4. having the potential to bioaccumulate (experimental BCF ≥ 100 or BMF >1 (or logPow ≥ 3, for organic substances only)) *plus* – classification as harmful or (very) toxic if swallowed or in contact with skin (R phrases R21, R22, R24, R25, R27 or R28); or – danger of serious damage to health by prolonged exposure (R48) The proposed EQS for Cd, Hg and Pb will be checked for compliance with the maximum permissible levels in fishery products seafood fixed by existing EU legislation (e.g. Council Regulation (EC) No 466/2001).	Derivation of an EQS referring to DW * abstraction only if the following cases apply (see section 4.3.3*** for details): 1. A 'A1 value' is fixed in Directive 75/440/EEC and this value is lower than the EQS for other objectives of protection: ⇒ EQS = 'A1 value' of CD 75/440/EEC 2. No 'A1 value' is fixed in CD 75/440/EEC but a DW Standard is available in CD 98/83/EC and the DWS ** is lower than the EQS for other protection objectives: ⇒ Assessment (Experts): Identification of the substance specific removal efficiency in DW processing. EQS = DWS / Fraction not removable 3. No A1 value or DW Standard exists for the substance concerned: ⇒ a) Calculation of a provisional DWS b) Assessment based on expert knowledge with regard to: 1. Removal efficiency of substance in DW processing; 2. Toxicological appropriateness of the provisional DWS EQS = appropriate DWS / Fract. not removable

* DW = drinking water; ** DWS = drinking-water standard; ***section 4.3.3. of FHI.

The following brief guidance can be extracted from these tables:

- Values for sediment and suspended matter are only derived if the substance adsorbs in significant amounts in these compartments: log $K_{p,\ susp\text{-}water} \geq 3$.
- When the selected BCF value is ≥ 100 or the final BMF value is > 1, MPCs for water addressing secondary poisoning and human fish consumption (provided that the substance is harmful or dangerous to humans) should be derived.
- When the final BCF value is < 100 or the final BMF value is ≤ 1, secondary poisoning needs not to be addressed. If the substance has CMR (carcinogenic, mutagenic, reprotoxic) properties, human fish consumption still has to be assessed. If not, this route too can be left aside. The BCF and BMF values are then not needed for MPC derivations. In this case, the collection of such data can be confined to a quick search in the databases.
- Note that when no experimental data on BCF or BMF values are available, a trigger value of log $K_{ow} \geq 3$ is used to decide whether an $MPC_{sp,\ water}$ (secondary poisoning) and an $MPC_{hh\ food,\ water}$ (human fish consumption) should be derived. Based on Eq. 6 which is developed for neutral organic compounds that are not metabolised, this log K_{ow} value leads to a BCF of 62. Therefore, this trigger value can be considered as a safe alternative if experimental BCF values are not available.

3.1.2 $MPC_{eco, water}$ – freshwater, ecotoxicity

3.1.2.1 Method of MPC derivation

The method derived in this section is valid for both organic substances and metals. After collection and tabulation of all relevant, useful and reliable toxicity studies, ERLs are derived. The method to derive the maximum permissible concentration (MPC) depends on the amount and type of available toxicity studies.

- When toxicity data for less than eight taxonomic groups according to the list of rules depicted in the TGD [p. 103] (see below which taxonomic groups) *or* less than ten species are available, the MPC is derived using assessment factors (section 3.1.2.2), equal to the preliminary effect assessment in the TGD. Data on field studies of mesocosms could provide an alternative way for deriving the MPC (see section 3.1.2.4). Where such data are available, the decision for selection of the final ERL is based on expert judgement.
- When toxicity data for at least eight taxonomic groups according to the list of rules depicted in the TGD [p. 103] (see below which taxonomic groups) *and* at least ten species (but preferably 15 species or more) are available, the MPC is derived using both the species sensitivity distribution (section 3.1.2.3), which is equal to the refined effect assessment in the TGD, *and* assessment factors. If data on field studies or mesocosms are available as well, an MPC is derived from these data if possible. The decision which of the two or three standards is taken as ERL is based on expert judgement.

However, with such a large diversity of data the use of statistical extrapolation is strongly recommended within the framework of INS. A valid reason for not using the statistical extrapolation method could be that the data do not follow a log-normal distribution.

The eight taxonomic groups that are required for the applicability of the refined effect assessment method are reported in the TGD. These taxonomic groups, prerequisite for applying the species sensitivity distribution, are shown below [cited from TGD, section 3.3.1.2., p. 103]:

1. Fish (species frequently tested include salmonids, minnows, bluegill sunfish, channel catfish, etc.);
2. A second family[19] in the phylum Chordata (fish, amphibian, etc.);
3. A crustacean (e.g. cladoceran, copepod, ostracod, isopod, amphipod, crayfish etc.);
4. An insect (e.g. mayfly, dragonfly, damselfly, stonefly, caddis fly, mosquito, midge, etc.);
5. A family in a phylum other than Arthropoda or Chordata (e.g. Rotifera, Annelida, Mollusca, etc.);
6. A family in any order of insect or any phylum not already represented[20];
7. Algae[21];
8. Higher plants.

3.1.2.2 MPC derivation using assessment factors (freshwater)

The MPC is derived by applying assessment factors according to the scheme shown in the TGD [section 3.3.1.1., p. 100-102, Table 16].

[19] INS addition: Some fish families that accommodate regularly tested species are: Salmonidae (a.o. all *Salmo* and *Oncorhynchus* sp.), Cyprinidae (a.o. *Carassius* sp., *Leuciscus* sp., *Brachydanio* sp., *Danio* sp., *Barbus* sp., *Rasbora* sp., *Phoxinus* sp.), Ictaluridae (*Ictalurus* sp.), Poeciliidae (a.o. *Poecilia* sp.) and Gasterosteidae (a.o. *Gasterosteus* sp.).
[20] INS addition: E.g. Bacteria, Protozoa, Cyanobacteria, Echinodermata, Coelerenterata, Cnidaria, etc.
[21] In the TGD, blue-green algae (cyanobacteria) are considered as algae (see TGD section 3.3.1.1 and Appendix IV). Therefore, when no valid data for green algae are available, these blue-green algae can complete the eight required taxonomic groups. The same phylum should then not represent the fifth or sixth bullet in the list.

The most important guidance for this scheme is that it should be interpreted as strictly as possible, taking notice of the text preceding Table 16 and the footnotes to Table 16 of the TGD. In this report, the scheme with assessment factors is shown in Table 18.

In this scheme, test species are grouped into trophic levels. The collection of acute toxicity tests which, at the simplest level, represents the aquatic ecosystem, consists of toxicity data for an algal species, a *Daphnia* species and a fish species. These organisms represent the trophic levels of primary producers, primary consumers and secondary consumers. The data set of acute toxicity data at three trophic levels is termed the base set.

Two important notes:
- The use of chronic toxicity data, and consequently an assessment factor of lower than 1000, is allowed only when at least the base set is complete (one reliable study for each of the trophic levels available).
- FHI guidance states: long-term annual average EQS (i.e. the MPC in INS framework) shall not be derived exclusively on the basis of acute toxicity data. This means that an MPC will not be derived when, in addition to a complete base set, no chronic toxicity data are available. This should be reported if MPC derivation is hampered by such a lack of data.

Citation from TGD [pp. 100-102]:
Table 18. Assessment factors to derive a $PNEC_{aquatic}$.

Available data	Assessment factor
At least one short-term L(E)C50 from each of three trophic levels of the base set (fish, *Daphnia* and algae)	1000 [a)]
One long-term NOEC (either fish or *Daphnia*)	100 [b)]
Two long-term NOECs from species representing two trophic levels (fish and/or *Daphnia* and/or algae)	50 [c)]
Long-term NOECs from at least three species (normally fish, *Daphnia* and algae) representing three trophic levels	10 [d)]
Species sensitivity distribution (SSD) method	5-1 (to be fully justified case by case) [e)]
Field data or model ecosystems	Reviewed on a case by case basis [f)]

Notes to Table 18:
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 uncertainties identified above 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 available evidence. A factor lower than 100 should not be used in deriving a PNECwater from short-term toxicity data except for substances with intermittent release (see section 3.3.2). There are cases where the base set is not complete: e.g. for substances that are produced at <1 t/a (notifications according to Annex VII B of Directive 92/32). 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)C50 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)C50 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)C50 of the short-term tests. This should, however, not apply in cases where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C50 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)C50 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 trophic level showing the lowest L(E)C50 in the short-term tests. This should however not apply in cases where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C50 of 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 PNECwater should be calculated from the lowest available 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[22].

e) Basic considerations and minimum requirements as outlined in Section 3.3.1.2.

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

Note that for INS purposes the species *Ceriodaphnia dubia* is considered to belong to the *Daphnia* species. This guidance has been added since both species are closely related; this increases the probability of completing the base set compared to the situation where only *Daphnia* would be accepted.

Not all details of the application of assessment factors are dealt with here. However, some attention must be paid to the following topics that are relevant on many occasions:
1. In preliminary effect assessment, species are grouped into trophic levels rather than taxonomic groups.
2. When the base set is complete, and only chronic toxicity data on algae are available; it is not allowed to apply an assessment factor of 100. If only chronic data for algae are available (in addition to a complete base set), the MPC is derived by applying an assessment factor of 1000 to the lowest acute test result (L(E)C50) from the base set.
3. If only one NOEC (or EC10) in addition to the base set is available, an assessment factor may only be applied to a NOEC (or EC10) for either *Daphnia* or fish (no other species).

[22] TGD guidance is incomplete here. We would like to add ‘unless enough valid data are available to construct a species sensitivity distribution (SSD)’. An SSD is also based on laboratory studies, with an assessment factor of 1 to 5 to be applied here.

4. An assessment factor of 100 is applied to the lowest chronic NOEC or EC10 if chronic data are available for only one trophic level of the base set, which has to be either *Daphnia* or fish. The lowest NOEC or EC10 should be from the same trophic level as that of the lowest acute L(E)C50. If this is not the case, a factor of 1000 is also applied to the lowest L(E)C50. The two results are compared: lowest L(E)C50/1000 versus NOEC (or EC10)/100; the lowest value is selected as ERL.
5. An assessment factor of 50 is applied to the lowest chronic NOEC, or EC10 if such chronic data are available from two trophic levels from the base set. The trophic levels of the NOECs and/or EC10s should include the trophic level of the lowest acute L(E)C50.
   If the trophic level of the lowest L(E)C50 is not included in that of the NOECs and/or EC10s then:
   - an assessment factor of 100 is applied to the lowest NOEC or EC10 if the lowest L(E)C50 is higher than the lowest NOEC or EC10;
   - an assessment factor of 100 is applied to the lowest L(E)C50 if the lowest L(E)C50 is lower than the lowest NOEC or EC10.
6. An assessment factor of 10 is applied to the lowest chronic NOEC or EC10 if chronic data are available from all three trophic levels of the base set. The trophic levels of NOECs and/or EC10s should include the trophic level of the lowest acute L(E)C50. If acute toxicity data are available for trophic levels not covered in the chronic toxicity data, and the trophic level of the lowest L(E)C50 is not included in that of the NOECs and/or EC10s then:
   - an assessment factor of 50 is applied to the lowest NOEC or EC10 if the lowest L(E)C50 is higher than the lowest NOEC or EC10;
   - an assessment factor of 100 is applied to the lowest L(E)C50 if the lowest L(E)C50 is lower than the lowest NOEC or EC10.
7. According to the TGD, data for bacteria are only used in the preliminary risk assessment as acute tests:
   'Micro-organisms 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' (cited from TGD). Consequently, NOECs or EC10 values derived from these studies may not be used in the derivation of MPCs using assessment factors, but EC50 values from bacterial tests may be used for MPC derivation. Data on bacteria are additional to the base set and can not be regarded as a substitution for any of the other trophic levels (acute data on algae, *Daphnia*, fish) for completion of the base set.
   In the section on the derivation of the PNEC for aquatic organisms, the TGD only refers to bacteria and micro-organisms and does not explicitly mention protozoans. However, in the section on the derivation of the PNEC for sewage treatment plants (STPs), bacteria and protozoans are referred to collectively as micro-organisms. Therefore, no assessment factor is applied to chronic tests with protozoans either.
   Please note (INS): NOECs or EC10 values from bacterial studies are valuable and should be tabulated amongst the toxicity data. They are relevant in the statistical extrapolation method (SSD) and derivation of SRC_{eco}.
8. Cyanobacteria (blue-green algae or Cyanophyta) belong to the trophic level of primary producers. This means that results from (both chronic and acute) tests with cyanobacteria can replace results with algae when applying the assessment factor scheme. Therefore, the results of these studies can be used to complete the base set, in cases where there is no study for algae. 'Additionally, blue-green algae should be counted among the primary producers due to their autotrophic nutrition' (cited from TGD).
9. If the base set is incomplete, but at least an acute toxicity study with *Daphnia* is available, the MPC is derived by applying an assessment factor of 1000 to the L(E)C50 for *Daphnia*. No guidance is available for cases where the base set is incomplete, and a *Daphnia* study is not

available. Hence, no MPC is derived following INS guidance when the base set is incomplete and when a short-term study with *Daphnia* is not available.

10. Further, the FHI guidance states that long-term annual average EQS (i.e. the MPC in INS framework) shall not be derived exclusively on the basis of acute toxicity data. This can be interpreted as: if no other routes are triggered (secondary poisoning, fish consumption and drinking water) to compare this value with, no environmental risk limits should be derived either.

3.1.2.3 MPC derivation using species sensitivity distributions

Guidance given in the TGD [section 3.3.1.2., p. 102-105] and the FHI document [section 4.3.4] should be followed when applying the species sensitivity distribution (SSD). Apart from species sensitivity distribution, the term statistical extrapolation is often used to describe the techniques that are discussed here.

Calculation of the SSD

All results from chronic toxicity studies, expressed as NOEC values or EC10 values, are collected. Results should be grouped in such a way that for each species only one entry is present (see section 2.2.6.1 for guidance on data handling). Freshwater and marine data are combined if allowed (see section 2.2.7.1 for guidance). Then the list of taxa and species required is checked to determine whether or not statistical extrapolation is allowed (see section 3.1.2.1 this document or TGD [section 3.3.1.2., p. 103]. The median HC_5 and its 90% confidence interval of the normal distribution (using log transformed concentrations) is calculated using the computer program *ETX* 2.0 (Van Vlaardingen *et al.*, 2004). The program is based on the method developed by Aldenberg and Jaworska (2000), which is the preferred method according to the FHI and INS guidance.

Both TGD and FHI also state that different statistical distributions may be used, however, only the log-logistic distribution is put forward as an example. Please note that the use of other distributions is favoured only after detailed analysis has shown that the log-normal distribution results in an inadequate fit (see next two sections). Moreover, other distributions may only be used if statistical uncertainty of the fit (at least goodness of fit and confidence interval around the estimated percentile) can be estimated with the software calculating the distributions.

Testing the goodness-of-fit of the SSD

The *ETX* 2.0 program also provides information on whether or not the data follow the log-normal distribution by means of three goodness-of-fit tests. The TGD states that 'the Anderson-Darling goodness-of-fit test can be used in addition to the Kolmogorov-Smirnov-test, as a criterion for the choice of a parametric distribution for comprehensive data sets, because it gives more weight to the tails of the distribution. A lack of fit may be caused by very different factors. One common factor seems to be the inclusion of several NOECs for species tested in a single laboratory, where the same test concentrations were used for all species. The statistical determination of the NOEC can lead to the same value being obtained for several species, showing up as a vertical row of NOECs in the cumulative distribution plots' (the reasons for not fitting a distribution can be very similar to the reasons why freshwater and marine data sets are different, see section 2.2.7.1). The (specific) mode of action of the investigated substance can be another reason for a lack of fit, causing species or groups of species to react more sensitively than expected on the basis of the selected distribution (next section).

Substances with a specific mode of action

'Another reason for lack of fit is a possible bimodality of the SSD, due to a specific mode of action of the tested substance towards only some taxonomic groups of species.' 'If the data do not fit any

distribution, the left tail of the distribution (the lowest effect concentrations) should be analysed more carefully. If a subgroup of species can be identified as particularly sensitive and if the number of data on this subgroup is sufficient, the distribution can be fit to this subgroup. In case of lack of fit, the SSD method should not be used.'

According to the guidance of the TGD, which is followed by FHI, an SSD on a subgroup of organisms, for example, insects, may only be applied after it has been shown that the overall distribution of the SSD, including all required taxonomic groups, shows a bimodality and if the number of data for the subgroup is sufficient. In both TGD and FHI guidance no further explanation is given on what is sufficient in this case. The initial requirement for the number of data is chronic toxicity data for at least ten (but preferably 15) species. Therefore, the number of species required to perform statistical extrapolation with a specific subgroup can be considered to be ten.

Deriving the MPC from the SSD
The section 'Estimation of the PNEC' is followed to determine the assessment factor that should be applied to the HC_5 in order to calculate the $MPC_{eco,\ water}$ [TGD, p. 105].

$$MPC_{eco,\ water} = PNEC = \frac{5\%SSD\ (50\%\ c.i.)}{AF} = \frac{HC_{5,\ median}}{AF} \qquad (9)$$

Notes:
1. This equation is cited from the TGD; the terms $MPC_{eco,\ water}$ and $HC_{5,\ median}$ are added for INS purposes.
2. 5% SSD (50% c.i.) stands for the median estimate of the 5th percentile of the SSD. The 5th percentile of the SSD is identical to the HC_5 (hazardous concentration at which 5% of the species are potentially affected), as shown in the last term of the equation.
3. In the FHI guidance, this value is referred to as P5-COV, which stands for 5-percentile cut-off value.

For the height of the assessment factor (AF) used, the TGD offers the following guidance
Citation from TGD [p. 105], also quoted in FHI [section 4.3.4]:
'AF is an appropriate assessment factor between 5 and 1, reflecting the further uncertainties identified. Lowering the AF below 5 on the basis of increased confidence needs to be fully justified. The exact value of the AF must depend on an evaluation of the uncertainties around the derivation of the 5th percentile. As a minimum, the following points have to be considered when determining the size of the assessment factor:
- the overall quality of the database and the endpoints covered, e.g., if all the data are generated from "true" chronic studies (e.g., covering all sensitive life stages);
- the diversity and representativeness of the taxonomic groups covered by the database, and the extent to which differences in the life forms, feeding strategies and trophic levels of the organisms are represented;
- knowledge on presumed mode of action of the chemical (covering also long-term exposure);
- statistical uncertainties around the 5th percentile estimate, e.g., reflected in the goodness of fit or the size of confidence interval around the 5th percentile, and consideration of different levels of confidence (e.g. by a comparison between the 5% of the SSD (50%) with the 5% of the SSD (95%));
- comparisons between field and mesocosm studies, where available, and the 5th percentile and mesocosm/field studies to evaluate the laboratory to field extrapolation.

A full justification should be given for the method used to determine the PNEC.'

The TGD states that all NOECs below the 5th percentile of the SSD should be discussed and examined to see if they belong to a particular sensitive group. That might be an indication that the underlying assumption of a normal distribution of the sensitivities is not met. Often, the assessment factor is chosen in such a way that the MPC is not much higher than the lowest NOEC found. However, with an increasing number of data, the chance of NOECs below the 5th percentile of the SSD becomes increasingly likely (e.g. with 20 NOECs, on average one value will be below the 5th percentile). This should be realised when discussing the NOECs below the 5th percentile.

3.1.2.4 MPC derivation using simulated ecosystem studies (micro/mesocosm)[23]

An MPC may also be derived from field data or model ecosystems. If such studies are available they should be included in the derivation of the MPC. However, the only guidance given in the TGD is that the assessment factor to be used on mesocosm studies or (semi-)field data will need to be reviewed on a case-by-case basis. In all cases, the MPC derived from mesocosm and semi-field studies should be compared with the other methods using assessment factors or statistical extrapolation.

Most of the simulated ecosystem studies are conducted under Council Directive 91/414/EEC (plant protection products). The FHI guidance adds to the guidance from the TGD that 'since the objectives of risk assessment under CD 91/414/EEC and the quality standards of the Water Framework Directive are not 100% compatible, it is necessary to carefully re-assess the results and conclusions of those studies for the purpose of quality standard setting'. What should be taken into account in this reassessment is summarised below.

- *The study in itself should be well performed and documented.*

FHI citation [p. 34, point 1]:
'It is essential that all relevant endpoints are addressed and the concentration of the active substance in the test system is monitored during the study in order to be able to calculate time-weighted average concentrations (C_{TWA}) for not fast dissipating active ingredients.'
End of citation
Since evaluation of these studies requires specific expert knowledge, guidance is not presented in this report. For guidance on the evaluation of micro- or mesocosm studies we refer to De Jong *et al*. (In prep.). However, it can be concluded from the FHI guidance that a first prerequisite for using a study is that the concentration of the substance is measured.

- *A long-term environmental risk limit should be based on average concentrations over a prolonged time interval.*

FHI citation [p. 34, point 2]:
'All effects observed (and all NOECs derived, respectively), must be related to the respective C_{TWA} in case a substance is not fast dissipating, in order to render the study results applicable for the derivation of a quality standard in the context of the WFD. It is not acceptable to use the initial concentration as reference.'
End of citation

The results of micro/mesocosm studies are mostly based on initial measured concentrations, because in the risk assessment of pesticides, it is presumed that the application on a field is a single event or repeated at several points in time, leading to a drop in concentration after application. However, larger water bodies that drain a wider agricultural area are exposed to more or less constant concentrations for a larger period of time. Therefore, the results from the mesocosm studies have to be expressed and recalculated on time-weighted average (TWA) concentrations. If

[23] The possibilities for the use of information from micro- and mesocosm studies in the derivation of environmental risk limits will be worked out in a separate study within the framework of INS.

this is not possible the studies can not be used for setting long-term environmental risk limits as the $MPC_{eco, water}$. The FHI document allows some exceptions for fast dissipating substances with a knock-down effect (e.g. certain carbamates or phosphoric acid esters). A study based on initial measured concentrations might still be useful for the derivation of the short-term $MAC_{eco, water}$.

- *An environmental risk limit should be based on no observed effects rather than the potential to recover.*

FHI citation [p. 35, point 3]:
'Absence of the occurrence of effects upon exposure to the prevailing substance concentration (either C_{TWA} or $C_{initial}$, depending on the dissipation and mode of action of the substance) rather than the potential to recover to the status quo ante within a certain time interval, e.g. 8 weeks, upon exposure to a single peak is the decisive criterion. The long-term quality standard (AA-EQS) in the context of the WFD refers by definition to an average concentration over a prolonged time interval. Hence, not the potential to recover after transient exposure but long-term undisturbed function and lack of impact on community structure of aquatic ecosystems at a prevailing average concentration level set by the EQS is the protection objective under the WFD.'
End of citation

Effects observed in micro/mesocosm studies are sometimes only transient. According to FHI the protection objective under the WFD implies that the absence of effects is the basis for the derivation of environmental risk limits rather than the potential for recovery. No explicit guidance on this topic is further given. If the Guidance Document on Aquatic Ecotoxicology in the context of the Directive 91/414/EEC (European Commission, 2002) is studied, this means that only class 1 ('effect could not be demonstrated') and possibly class 2 ('slight effect') are accepted, provided that the effects are not dose-related and observed at individual samplings only. The effect concentrations from micro- or mesocosm studies at which effects are excluded (restricted to the study and based on statistical techniques) are the $NOEC_{community}$ and/or $NOEC_{population}$.

According to the Guidance Document on Aquatic Ecotoxicology (European Commission, 2002), the environmentally acceptable concentration (EAC) is derived from the no observed ecologically adverse effect concentration (NOEAEC) by applying an appropriate uncertainty factor. The NOEAEC is again derived from the microcosm, mesocosm or field study. A classification for effects is given in the guidance document for plant protection products. The NOEAEC may be higher than the lowest NOEC in the study, provided that the effects are temporary. Further, the NOEAEC is based on initial concentrations in the study. The assessment factor to derive the EAC from this NOEAEC is dependent on the severity of these transient effects. FHI concludes that the EAC in the Guidance Document on Aquatic Ecotoxicology serves a different protection level than the PNECs for industrial chemicals according to the TGD and long-term environmental risk limits that are derived within the Water Framework Directive.

- *To obtain an environmental risk limit the results from one or more studies should be extrapolated to all water bodies.*

FHI citation [p. 35, point 5]:
'The scope of protection of an environmental quality standard under the WFD is broader than that of the 'acceptable concentration' in the PPP-RA. In deriving a surface water quality standard from a Higher-Tier simulated ecosystem study it is therefore indispensable to consider that the quality standard must be protective for all types of surface waters and communities that are addressed by the respective standard, as long as it is not possible to rule out that exposure to plant protection products may occur in particular types of water bodies. This means that in the interpretation of Higher-Tier studies, an evaluation is necessary as to whether the test system and the tested community, respectively, can be considered as representative for all water bodies that potentially are subject to PPP exposure. Higher-Tier studies in the context of the PPP-RA are normally focused

to eutrophic shallow water bodies usually occurring in the immediate vicinity of agriculturally used areas. An EQS under the WFD, however, must assure protection also for water bodies that significantly differ from this paradigm, such as those having different flow regimes or trophic status, for instance.'
End of citation

The citation above focuses specifically on plant protection products. However, in the INS framework, this guidance is expanded to all substances for which micro- or mesocosm studies are evaluated for ERL derivation, since these studies are not restricted to PPPs only. The FHI guidance illustrates the differences between the risk assessment for the ditch at the edge of the field and the derivation of environmental risk limits for larger water bodies. Most freshwater micro- or mesocoms studies are mesotrophic. However, in the derivation of the environmental risk limits all types of surface water and communities where the pesticide may occur, should be protected. FHI signals that the derived standard should assure protection of all water bodies that are potentially subject to exposure to the substance. To this end, an evaluation should take place to assess whether the results obtained from the available micro- or mesocosm studies can be extrapolated to all water bodies that are to be protected by the $MPC_{eco,\ water}$. This should be reflected in a proper assessment factor, which is subject to expert judgement according to FHI. The height of this assessment factor is not given by FHI. Therefore, it is proposed in the framework of INS to apply a similar assessment factor as applied to the results of the statistical extrapolation method. The following is thus the INS guidance.

$$MPC_{eco,\ water} = \frac{\min\left\{NOEC_{community},\ NOEC_{population}\right\}}{AF} \qquad (10)$$

The $MPC_{eco,\ water}$ is determined by applying an assessment factor to the lowest NOEC determined in micro- or mesocosm studies, represented by $\min\{NOEC_{community}, NOEC_{population}\}$ in equation 10. The height of the assessment factor (AF) may vary from 1 to 5.
To determine the height of the assessment factor, an expert should be consulted. Consider the following topics:

- The overall quality of the micro- or mesocosm study/studies from which the NOEC has been derived.
- The relationship between the mode of action of the investigated substance and the species represented in the available micro- or mesocosm studies.
- Do the available micro- or mesocosm studies cover vulnerable species or representatives of taxonomic groups (e.g. families, orders) of vulnerable species that are part of the aquatic ecosystems to be protected?
- Do the available micro- or mesocosm studies represent the range of flow regimes that should be protected by the $MPC_{eco,\ water}$? Consider specific populations of species inhabiting the lotic and lentic water types to be protected.
- Do the available micro- or mesocosm studies represent the range of trophic statuses of water bodies that should be protected by the $MPC_{eco,\ water}$?

3.1.3 $MPC_{eco,\ marine}$ – marine water, ecotoxicity

According to the FHI guidance, the $MPC_{eco,\ water}$ for freshwater can be considered valid for inland waters, both for metals and organic substances. $MPC_{eco,\ marine}$ is valid for transitional and marine (coastal and territorial) waters. The MPC for marine water ($MPC_{eco,\ marine}$) is derived by applying assessment factors according to the scheme shown in the TGD [section 4.3.1.3., p. 148-151, Table 25].

Citation TGD [pp. 149-150]:

Table 19. Assessment factors proposed for deriving PNECwater for saltwater for different data sets.

Data set	Assessment factor
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10,000 [a)]
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels, + two additional marine taxonomic groups (e.g. echinoderms, molluscs)	1000 [b)]
One long-term NOEC (from freshwater or saltwater crustacean reproduction or fish growth studies)	1000 [b)]
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish)	500 [c)]
Lowest long-term NOECs from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels	100 [d)]
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish) + one long-term NOEC from an additional marine taxonomic group (e.g. echinoderms, molluscs)	50
Lowest long-term NOECs from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels + two long-term NOECs from additional marine taxonomic groups (e.g. echinoderms, molluscs)	10

Notes to Table 19:
Evidence for varying the assessment factor should in general include a consideration of the availability of data from a wider selection of species covering additional feeding strategies/ life forms/ taxonomic groups other than those represented by the algal, crustacean and fish species (such as echinoderms or molluscs). This is especially the case, where data are available for additional taxonomic groups representative of marine species. More specific recommendations as with regard to issues to consider in relation to the data available and the size and variation of the assessment factor are indicated below.
When substantiated evidence exists that the substances may be disrupting the endocrine system of mammals, birds, aquatic or other wildlife species, it should be considered whether the assessment factor would also be sufficient to protect against effects caused by such a mode of action, or whether an increase of the factor would be appropriate.

a) The use of a factor of 10,000 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 identified uncertainties described above 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, as defined in Section 2.3.3.4, under no circumstances should a factor lower than 1000 be used in deriving a PNECwater for saltwater from short-term toxicity data.
Evidence for varying the assessment factor could include one or more of the following:
- evidence from structurally similar compounds which may demonstrate that a higher or lower factor may be appropriate.
- knowledge of the mode of action as 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 higher factor.
- 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 multiple data points are

available for the most sensitive taxonomic group (i.e. the group showing acute toxicity more than 10 times lower than for the other groups).

There are cases where a complete short-term dataset even for freshwater algal, crustacean and fish species will not be available, for example for substances which are produced at < 1 t/a (notifications according to Annex VII B of Directive 92/32). In these situations, the only data may be short-term L(E)C50 data for Daphnia. In these exceptional cases, the PNEC should be calculated with a factor of 10,000.

Variation from an assessment factor of 10000 should be fully reported with accompanying evidence.

b) An assessment factor of 1000 applies where data from a wider selection of species are available covering additional taxonomic groups (such as echinoderms or molluscs) other than those represented by algal, crustacean and fish species; if at least data are available for two additional taxonomic groups representative of marine species.

An assessment factor of 1000 applies to a single long-term NOEC (freshwater or saltwater crustacean or fish) if this NOEC was generated for the taxonomic group showing the lowest L(E)C50 in the short-term algal, crustacean or fish tests.

If the only available long-term NOEC is from a species which does not have the lowest L(E)C50 in 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 10,000. However, normally the lowest PNEC should prevail.

An assessment factor of 1000 applies also to the lowest of the two long-term NOECs covering two trophic levels (freshwater or saltwater algae and/or crustacean and/or fish) when such NOECs have not been generated for the species showing the lowest L(E)C50 of the short-term tests.

This should not apply in cases where the acutely most sensitive species has an L(E)C50-value lower than the lowest NOEC value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest L(E)C50 of the short-term tests.

c) An assessment factor of 500 applies to the lowest of two NOECs covering two trophic levels (freshwater or saltwater algae and/or crustacean and/or fish) when such NOECs have been generated covering those trophic levels showing the lowest L(E)C50 in the short-term tests with these species. Consideration can be given to lowering this factor in the following circumstances:

- It may sometimes be possible to determine with a high probability that the most sensitive species covering fish, crustacea and algae has been examined, that is that a further longer-term NOEC from a third taxonomic group would not be lower than the data already available. In such circumstances an assessment factor of 100 would be justified;
- a reduced assessment factor (to 100 if only one short-term test, to 50 if two short-term tests on marine species are available) applied to the lowest NOEC from only two species may be appropriate where:
  − short-term tests for additional species representing marine taxonomic groups (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and;
  − it has been determined with a high probability that long-term NOECs generated for these marine groups would not be lower than that already obtained. This is particularly important if the substance does not have the potential to bioaccumulate.

An assessment factor of 500 also applies to the lowest of three NOECs covering three trophic levels, when such NOECs have not been generated from the taxonomic group showing the lowest L(E)C50 in short-term tests. This should, however, not apply in the case where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by
applying an assessment factor of 1000 to the lowest L(E)C50 in the short-term tests.

d) An assessment factor of 100 will be applied when longer-term toxicity NOECs are available from three freshwater or saltwater species (algae, crustaceans and fish) across three trophic levels.

The assessment factor may be reduced to a minimum of 10 in the following situations:

- where short-term tests for additional species representing marine taxonomic groups (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and it has been determined

with a high probability that long-term NOECs generated for these species would not be lower than that already obtained;
- where short-term tests for additional taxonomic groups (for example echinoderms or molluscs) have indicated that one of these is the most sensitive group acutely and a long-term test has been carried out for that species. This will only apply when it has been determined with a high probability that additional NOECs generated from other taxa will not be lower than the NOECs already available.

A factor of 10 cannot be decreased on the basis of laboratory studies only[24].'
End of citation

Attention should be paid to the following points:
1. The most important guidance on Table 19, is that it should be interpreted as strictly as possible, taking notice of the TGD text preceding this scheme [TGD, p. 148-149] and the footnotes to Table 19. The FHI states the following:
   FHI citation
   'Thus, where only data for freshwater or saltwater algae, crustaceans and fish are available a higher assessment factor than that used for the derivation of the inland water (freshwater) quality standard should be applied to reflect the greater uncertainty in the extrapolation. Where data is available for additional marine taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a data set can be lowered.'
   'Thus, an additional assessment factor is not automatically applied in the effects assessment and quality standard setting procedure referring to transitional, costal and territorial waters. This additional AF is only used if the available data do not appropriately represent the communities that dwell in the addressed marine ecosystems. If marine life forms are sufficiently represented in the data set available, the recommended assessment factors do not differ from those used in the freshwater effects assessment.'
   End of citation
2. ERLs for marine water (and freshwater) should be derived on the basis of distinct data sets only when toxicity data sets for marine and freshwater organisms can not be combined (see section 2.2.7.1 for guidance). In most cases, however, toxicity data sets for freshwater and marine organisms can be combined for ERL derivation.
3. For metals and pesticides (plant protection products), in general, the data for freshwater and saltwater must not be pooled (see section 2.2.7.1, page 57). However, if there is strong evidence that pooling of the sets is justified, this might be considered.
4. In the case that freshwater and marine toxicity data should not be combined and the marine data set is so extensive that statistical extrapolation is possible, the MPC should be derived using statistical extrapolation as described for freshwater in section 3.1.2.3 of this report. Otherwise, the derivation of the MPC should be performed on the basis of assessment factors, taking only the marine data into account.
5. *Additional INS guidance*. However, the following exceptional case can occur. A statistical comparison shows that there is a difference in sensitivity between freshwater organisms and saltwater organisms. However, due to the use of different assessment factors, the compartment with the more sensitive organisms ends up with a higher MPC than the compartment with the less sensitive organisms. Generally, such a situation should be prevented. In such cases, consider using the lowest value for both compartments, or to use the same assessment factor for both data sets.

[24] See footnote 22 at page 72.

The FHI guidance gives some additional information on the use of statistical extrapolation for the derivation of risk limits for the marine environment. For combining data sets (freshwater and marine), the same considerations apply as stated for the derivation of risk limits with the assessment factor method.

Citation from FHI, page 30-31.
'The same assessment factor on the result of the SSD (the 5% cut-off value) than considered appropriate for inland waters (see section 4.3.4) should however only be applied for transitional, coastal and territorial waters if the data set used to establish the SSD comprises long-term NOECs of at least 2 additional marine taxonomic groups other than fish, crustaceans and algae (e.g. echinoderms, molluscs, coelenterata), showing that these additional marine groups are not more sensitive than other taxa. Where this cannot be proven, or otherwise be established that marine organisms are not more sensitive, an additional assessment factor of 10 on the EQS referring to inland waters may be used to derive the corresponding EQS for transitional, coastal and territorial waters.
Where the hypothesis of a reasonable correlation between ecotoxicological responses of freshwater and saltwater biota cannot be justified based on the available evidence, SSD based EQS for inland surface waters and transitional, coastal and territorial waters must be derived on the basis of distinct data sets for freshwater and marine organisms, respectively. For setting up the SSD with ecotoxicological data of marine organisms the same data requirements regarding the quantity and quality of input data as laid down in section 4.3.4.1 (of FHI, see section 3.1.2.1 in this document) apply. However, with regard to the species requirements laid down in table 10 (of FHI, see section 3.1.2.1 in this document), insects and higher plants may be replaced by more typical marine taxa such as, e.g., molluscs, echinoderms or coelenterata.'
End of citation

3.1.4 $MPC_{sp,\ water}$ and $MPC_{sp,\ marine}$ – secondary poisoning

3.1.4.1 Introduction

Secondary poisoning should be assessed when BCF ≥ 100 or BMF >1. If a reliable BCF is not available, secondary poisoning should be assessed if log $K_{ow} \geq 3$ (for organic substances only). Guidance on secondary poisoning as given in FHI [section 4.3.2.5., p. 23] follows the TGD [sections 3.8.3, p.124 and 4.3.3, p. 157]. However, while the TGD follows the route from a PEC_{water} towards a risk quotient for a (top) predator (bird or mammal), the FHI follows the opposite route. From a safe level for a (top) predator (bird or mammal), a safe water concentration is calculated. Dissimilarities between the two guidance documents in terminology of parameters and their units are shown in Table 20. For the freshwater compartment, the TGD and the FHI document describe the route from aquatic organisms, via biomagnification in fish, to a fish eating predator (bird or mammal). The assumption is that the concentration in the food of the predator (fish) is equal to NOEC in food from the laboratory experiments with birds or mammals.

Table 20. Parameters used in secondary poisoning guidance in TGD and FHI; dissimilarities.

TGD	Unit	FHI	Unit
PEC_{water}	$mg.L^{-1}$	$QS_{secpois\ water}$	$\mu g.L^{-1}$
$PNEC_{oral}$	$kg.kg_{food}^{-1}$	$QS_{secpois\ biota}$	$\mu g.kg^{-1}$

3.1.4.2 Freshwater, derivation of $MPC_{sp,\ water}$

The $MPC_{sp,\ water}$ for the freshwater compartment is calculated as follows:

1. Convert all $NOEC_{bird}$ and $NOEC_{mammal,\ food\_chr}$ values (=TOX_{oral} in $\mu g.kg_{food}^{-1}$ or $mg.kg_{food}^{-1}$) to $MPC_{oral,\ bird}$ and or $MPC_{oral,\ mammal}$ values by applying an assessment factor according to Table 21 and Eqs. 11 and 12.

$$MPC_{\text{oral, bird}} = \frac{TOX_{\text{oral}}}{AF_{\text{oral}}} \quad (11)$$

$$MPC_{\text{oral, mammal}} = \frac{TOX_{\text{oral}}}{AF_{\text{oral}}} \quad (12)$$

Table 21. Assessment factors for extrapolation of mammalian and bird toxicity data.

TOX_{oral}	Duration of test	AForal
LC50 bird	5 days	3000
NOECbird	chronic	30
NOECmammal, food_chr	28 days	300
	90 days	90
	chronic	30

2. Select the *lowest* of the MPC_{oral} values for different species for calculating the $MPC_{sp, water}$. According to the FHI guidance, the statistical extrapolation method could be used as well if enough data for birds and mammals are available. However, no criteria for the quality and quantity of such data are available (FHI document, footnote 11 on page 27). If the same requirement as for aquatic organisms is applied to birds and mammals, this would imply a number of at least 10 species. No explicit guidance is given in FHI and TGD on how to deal with data for one species from several studies. However, if for the same species more than one study is available, it seems logical to use the most sensitive endpoint divided by the appropriate assessment factor (i.e. the factor implied by the study with the longest test duration).
3. Calculate the $MPC_{sp, water}$ using Eq. 13:

$$MPC_{\text{sp, water}} = \frac{MPC_{\text{oral, min}}}{BCF_{\text{fish}} \cdot BMF_1} \quad (13)$$

In addition, when a BCF value for mussels is available, calculate $MPC_{sp, water}$ according to Eq. 13 by replacing BCF_{fish} by BCF_{mussel}. The TGD gives guidance on the inclusion of data for mussels; see TGD [section 3.8.3.1, page 125] and TGD [section 4.3.3.2, page 159]. In the FHI guidance, the route via mussels is also mentioned for both the freshwater and marine compartment (FHI: Table 2, page 13). In this route a biomagnification step from mussels to fish is included, which might be taken equal to the biomagnification factor from small to larger fish. However, because the mussels may serve as prey for mammals and birds directly, the biomagnification factor might be omitted. This can be relevant in the cases where the biomagnification factor from mussel to fish is lower than 1 due to the higher metabolic capacity of fish compared to mussels for that specific compound. In the bioaccumulation step from water to mussels, bioconcentration in algae and biomagnification from algae to mussels are not addressed separately. As addressed in section 2.3.2, BCF data for algae must be considered as unreliable. This biomagnification step may indirectly be included in the risk assessment if the used BCF value for mussels is determined in a study, in which the mussels were fed with algae.

3.1.4.3 Marine water, derivation of $MPC_{sp, marine}$

The $MPC_{sp, marine}$ is calculated in a manner identical to that for the freshwater compartment. To calculate $MPC_{sp, marine}$, follow section 3.1.4.2., step 1 and 2. Step 3 of that section is replaced by the following.

To account for the longer food chains in the marine environment, the route from water to top predator is extended with one extra biomagnification step. This step represents the biomagnification

from fish to fish-eating birds and mammals that serve as prey for top predators. Thus the route of exposure is uptake by aquatic organisms (e.g. small fish), biomagnification by fish, biomagnification by fish-eating predators and finally, consumption by the top predator. The equation that corresponds with this food chain is described by Eq. 14:

$$MPC_{\text{sp, marine}} = \frac{MPC_{\text{oral, min}}}{BCF_{\text{fish}} \cdot BMF_1 \cdot BMF_2} \qquad (14)$$

In addition, when a BCF value for mussels is available, calculate $MPC_{\text{sp, water}}$ according to Eq. 14 by replacing BCF_{fish} by BCF_{mussel}.

Both the FHI document and the TGD give the same default values for the biomagnification factors. These BMF values and their selection method are reported in Table 12 in section 2.3.4.4. Selection of BCF values is described in sections 2.3.4.1 and 2.3.4.2. For metals the same TGD-based approach should, in principle, be followed as for organic substances.

3.1.5 $MPC_{\text{hh food, water}}$ – human consumption of fishery products

Uptake of compounds via human consumption of fishery products should be assessed when the classification of the compound of interest includes one or more of the R phrases tabulated in Table 17 (under Biota (Food consumption)). The $MPC_{\text{hh food, water}}$ is calculated according to Eqs. 15 and 16 from the threshold level (TL_{hh}) for humans, *viz*. ADI, TDI or $NO(A)EL_{\text{oral}}$ (the latter divided by a proper assessment factor (see [Table 2 of the FHI document] or Eq. 19 of this report). In this calculation, the contribution of consumption of fishery products to the threshold level is at most 10%. Further, a body weight of 70 kg and a daily consumption of fish of 115 g are assumed.

$$MPC_{\text{hh, food}} = \frac{0.1 \cdot TL_{hh} \cdot BW}{0.115} \qquad (15)$$

$$MPC_{\text{hh food, water}} = \frac{MPC_{\text{hh, food}}}{BCF_{\text{fish}} \cdot BMF_1} \qquad (16)$$

See section 2.4 for the selection procedure of the parameter TL_{hh}, which is a human toxicological risk limit. According to the FHI document, both fish and mussels belong to the category of fishery products. The BCF in Eq. 16 may thus be a BCF for fish as well as for mussels (see 3.1.4.2 for further guidance).

Although the additional effect of biomagnification is considered relevant for secondary poisoning by the TGD, it is not mentioned in the risk assessment for humans exposed through fish consumption (European Commission (Joint Research Centre), 2003c). The guidance of FHI can be considered as a valid improvement with regard to the TGD.

The $MPC_{\text{hh food, water}}$ is valid for the freshwater as well as for the marine compartment.

3.1.6 $MPC_{\text{dw, water}}$ – drinking-water abstraction

A second route for human exposure to compounds in water is the abstraction of drinking water. The $MPC_{\text{dw, water}}$ is derived in the following way [FHI section 4.3.3]:

1. If an A1 value (see section 3.1, Table 17 and/or Appendix 1) is available, the $MPC_{dw, water}$ will be set equal to the A1 value.
2. If no A1 value is available but a DW standard is available (from CD 98/83/EC, see section 3.1, Table 17 and/or Appendix 2), follow the procedure described below:
   - If the DW standard is higher than the other MPC_{water} values already derived (*viz*. $MPC_{eco, water}$, $MPC_{sp, water}$, $MPC_{hh\ food, water}$), the procedure stops. A quality standard for drinking-water abstraction need not be derived.
   - If the DW standard is lower than the other MPC_{water} values already derived (*viz*. $MPC_{eco, water}$, $MPC_{sp, water}$, $MPC_{hh\ food, water}$), a quality standard for drinking-water abstraction ($MPC_{dw, water}$) by simple treatment (Category A1 in CD 75/440/EEC) is derived as follows:.
     – Drinking-water experts are consulted in order to predict substance specific removal efficiencies of simple surface water treatment. Express the removal efficiency as a *fraction not removable by simple treatment*.
     – The $MPC_{dw, water}$ is calculated with Eq. 17.

$$MPC_{dw, water} = \frac{DW\ \text{standard (CD 98/83/EC)}}{F_{\text{not removable by simple treatment}}} \qquad (17)$$

3. If no A1 value is available and no DW standard is available, follow the procedure described below:
   - A provisional drinking-water standard is calculated according to Eq. 18. This calculation by FHI [section 4.3.3] is based on recommendations of the TGD [part I, section 2.4.3 and Appendix III].

$$MPC_{dw, water, provisional} = \frac{0.1 \cdot TL_{hh} \cdot BW}{Uptake_{dw}} \qquad (18)$$

According to the TGD, the human body weight (*BW*) is 70 kg, the daily uptake of drinking water 2 L. According to FHI, the value for TL_{hh} should be the ADI or TDI if these are available.
If no ADI or TDI is available, the TL_{hh} is calculated from the $NOEL_{min}$ using Eq. 19:

$$TL_{hh} = NOAEL_{oral, human} = \frac{NOEL_{min}}{100} \qquad (19)$$

If the compound of interest is potentially carcinogenic[25], the TL_{hh} is equal to the concentration corresponding to an additional risk of cancer 1×10^{-6} (for 70 years exposure). See section 2.4.1 for the selection procedure of the parameter TL_{hh}.

   - If the (provisional) drinking-water standard is higher than the other MPC_{water} values already derived (*viz*. $MPC_{eco, water}$, $MPC_{sp, water}$, $MPC_{hh\ food, water}$), the procedure stops. A quality standard for drinking-water abstraction need not be derived.
   - If the $MPC_{dw, water, provisional}$ calculated using Eq. 18 is lower than the other MPC_{water} values already derived (*viz*. $MPC_{eco, water}$, $MPC_{sp, water}$, $MPC_{hh\ food, water}$), a quality standard for drinking-water abstraction ($MPC_{dw, water}$) by simple treatment (Category A1 in CD 75/440/EEC) is derived following the two steps described below.
     – Drinking-water experts are consulted in order to predict substance specific removal efficiencies of simple surface water treatment. Express the removal efficiency as a fraction

[25] No guidance is given on how to establish the potential carcinogenicity of a compound. We propose checking the appropriate R phrases. No guidance is given either on how to arrive at a level of 10^{-6} unit risk value for cancer.

not removable by simple treatment.
– The $MPC_{dw, water}$ is calculated with Eq. 16.

For metals, the same approach as described for organic chemicals is followed.

3.1.7 Selection of the final MPC for the water compartment

3.1.7.1 MPC_{water} – freshwater

A series of MPC values for the freshwater compartment have now been derived. The number of MPC values available depends on the characteristics of the compound and on data availability. The following MPC_{water} values can potentially be derived:

$MPC_{eco, water}$	MPC_{water} based on ecotoxicological data
$MPC_{sp, water}$	MPC_{water} based on secondary poisoning
$MPC_{hh\ food, water}$	MPC_{water} based on human consumption of fishery products
$MPC_{dw, water}$	MPC_{water} for drinking-water abstraction

1. The final value for the MPC_{water} is the lowest value of the available MPC values [FHI, page 3 and page 9].
2. According to FHI guidance, any of the above calculated MPCs is assumed to reflect a total water concentration ('total' meaning the dissolved concentration + concentration sorbed to suspended particulate matter). Hence, the final quality standard in water for organic substances refers to the total concentration in unfiltered water. Recalculation of standards from dissolved to total water concentrations at the end of the derivation procedure, which has been standard procedure in INS framework, is therefore no longer necessary under the current guidance.[26]
3. For metals however, the quality standard refers to the dissolved concentration in filtered water samples (FHI guidance). For metals this is worked out by stating that in toxicity experiments the added part of the metal is fully bioavailable. We refer to section 3.1.8 for the method to calculate total concentrations.

3.1.7.2 MPC_{marine} – marine water

The overall MPC for the marine environment (MPC_{marine}) should in principle be based on the same procedure. However, no specific guidance on this subject is given in the FHI guidance. Of the series of MPC values derived for the freshwater compartment, only drinking-water abstraction is mostly not relevant for the marine environment, although there are exceptional cases in which saltwater is used for preparation of drinking water. In general, the lowest value of the other three routes should be chosen as MPC for marine water. The number of MPC values available depends on the characteristics of the compound and on data availability. The following MPC_{water} values can potentially be derived:

$MPC_{eco, marine}$	MPC_{water} based on ecotoxicological data
$MPC_{sp, marine}$	MPC_{water} based on secondary poisoning
$MPC_{hh\ food, water}$	MPC_{water} based on human consumption of fishery products

The final value for the MPC_{marine} is the lowest value of the available MPC values.

[26] In well-performed aquatic toxicity studies as well as in valid BCF studies, the amount of suspended matter should be negligible. This means that the substance is fully dissolved. These types of studies form the basis for all routes of deriving risk limits, except drinking-water abstraction. Indeed, in risk assessment reports of the EU, the predicted environmental concentration, which is compared with the PNEC, is based on dissolved concentrations (Janssen *et al.*, 2004). This reasoning applies, in principle, to all substances and not only to metals. However, under the Water Framework Directive only one value is derived based on the presented guidance, which represents the total concentration of organic substances in water.

3.1.8 Calculation of the MPC in suspended matter

Following FHI guidance, the final MPC_{water} has to be reported as $MPC_{water, total}$ and in addition, if log $K_{p, susp\text{-}water} \geq 3$, as the $MPC_{susp, water}$. $MPC_{susp, water}$ refers to the concentration in suspended particulate matter. Equations for its derivation are given in the following sections. The MPC values for fresh and marine water are derived using the same methodology and equations. A suspended matter concentration of 3 mg.L^{-1} in seawater is used in this calculation (instead of 30 mg.L^{-1} for freshwater, see Table 2).

3.1.8.1 Organic compounds

For organic compounds with log $K_{p, susp\text{-}water} \geq 3$, MPC values have to be reported as $MPC_{susp, water}$, this is the concentration in suspended particulate matter.

Freshwater

The concentration in suspended particulate matter is calculated from the MPC for the total concentration in water by means of Eq. 20 [FHI guidance]:

$$MPC_{susp,\ water} = \frac{MPC_{water,\ total}}{C_{susp,\ Dutch\ standard} \times 10^{-6} + \frac{1}{K_{p,\ susp-water}}} \qquad (20)$$

In this equation, the characteristics for Dutch standard suspended matter should be chosen: $C_{susp\ Dutch\ standard}$ = 30 mg.L^{-1} and $Foc_{Dutch\ standard\ susp}$ = 11.76 % (see Table 31 and/or Table 2).

Marine water

The concentration in suspended particulate matter is calculated from the MPC for the total concentration in marine water by means of Eq. 21 [FHI guidance]:

$$MPC_{susp,\ marine} = \frac{MPC_{marine,\ total}}{C_{susp\ marine,\ FHI} \times 10^{-6} + \frac{1}{K_{p,\ susp-water}}} \qquad (21)$$

In this equation, the FHI concentration of suspended matter in marine water is chosen: $C_{susp\ marine,\ FHI}$ = 3 mg.L^{-1} (a Dutch standard value is not available) and $Foc_{Dutch\ standard\ susp}$ = 11.76 %.

3.1.8.2 Metals

Recalculation of $MPC_{water, dissolved}$ into $MPC_{water, total}$ for metals is performed using the same methodology as described in the previous section. However, since the added risk approach is followed (see section 3.6), the procedure is slightly different. Guidance from FHI is summarised in the following procedure:

1. Based on the toxicity data available, the $MPA_{water, dissolved}$ is derived.
2. The $MPA_{water, total}$ is calculated using Eq. 22:

$$MPA_{water,\ total} = MPA_{water,\ dissolved} \times (1 + K_{p,\ susp-water} \times 10^{-6} \times C_{susp,\ Dutch\ standard}) \qquad (22)$$

3. Eq. 23 is used to calculate an $MPA_{water, susp}$. Here the FHI guidance adds that the partition coefficient used needs to be a locally relevant partition coefficient, because the $K_{p, susp\text{-}water}$ is highly dependent on local water quality conditions.

$$MPA_{\text{water, susp}} = MPA_{\text{water, dissolved}} \times K_{\text{p, susp–water}} \quad (23)$$

4. If the background concentration (C_b) of the metal for which the MPC is going to be derived is available as total concentration, recalculate this value to $C_{\text{b, dissolved}}$ for use in Eq. 24. To this end, rearrange Eq. 22 and substitute MPA by C_b.
5. If the background concentration (C_b) of the metal for which the MPC is going to be derived is available as dissolved concentration, recalculate this value to $C_{\text{b, total}}$ for use in Eq. 25. To this end, use Eq. 22 and substitute MPA by C_b.
6. If an $MPC_{\text{susp, water}}$ has to be reported, calculate $C_{\text{b, susp}}$ using Eq. 24.

$$C_{\text{b, susp}} = C_{\text{b, dissolved}} \times K_{\text{p, susp–water}} \quad (24)$$

7. The final MPCs for metals are then calculated as follows:

$$MPC_{\text{water, total}} = C_{\text{b, total}} + MPA_{\text{water, total}} \quad (25)$$

$$MPC_{\text{water, susp}} = C_{\text{b, susp}} + MPA_{\text{water, susp}} \quad (26)$$

3.2 Sediment compartment

3.2.1 $MPC_{sediment}$ – freshwater

3.2.1.1 MPC derivation using assessment factors

The FHI guidance should be followed for the derivation of the $MPC_{sediment}$:

- When no toxicity test results are available for sediment organisms, the equilibrium partitioning method (EqP) is applied to calculate the $MPC_{sediment}$ from $MPC_{eco, water}$. The EqP method is worked out in section 3.7. In the case that the log K_{ow} value of the test substance is higher than 5, an extra assessment factor of 10 is applied to the value calculated by equilibrium partitioning to account for the (possible) role of food ingestion;
- When only acute toxicity test results for benthic organisms are available (FHI: 'a marginal short-term effects database'), the risk assessment is performed both on the basis of the test result of the most sensitive species using an assessment factor of 1000 *and* on the basis of the equilibrium partitioning method. In contrast to the principle adopted for the aquatic compartment, it is not necessary to have three acute sediment tests for the assessment factor of 1000 to be applicable [TGD, section 3.5.4]. The $MPC_{sediment}$ is then set based on expert judgement[27] taking all available information into account;
- When long-term toxicity test data are available for benthic organisms, the $MPC_{sediment}$ is calculated using assessment factors for long-term tests and this result should prevail in the risk assessment. The appropriate assessment factors are given in Table 22. The assessment factor is lowered only with each additional species representing different living and feeding conditions.

[27] Please note that FHI overrules TGD guidance at this point. Therefore, the TGD guidance 'the lowest $MPC_{sediment}$ is then used for the risk characterisation' no longer applies in a strict sense, but might still be useful as a rule of thumb.

FHI and TGD citation:

Table 22. Assessment factors for derivation of $MPC_{sediment}$.

Available test result	Assessment factor
One long term test (NOEC or EC10)	100
Two long term tests (NOEC or EC10) with species representing different living and feeding conditions	50
Three long term tests (NOEC or EC10) with species representing different living and feeding conditions	10

End of citation

According to FHI guidance an $MPC_{sediment}$ value which is not based on at least three chronic benthic toxicity data with sediment organisms representing different life and feeding conditions, should be considered as an indicative value.

The added risk approach for metals (section 3.6) also applies to sediment. The FHI guidance states that this method should be used with a locally relevant background concentration in order to derive local quality standards. Preliminary effect assessment is applied to data for sediment organisms following the same methodology as for organic substances. In the FHI main report (Lepper, 2002), [in section 8.6.5 (p. 91 and 92)] it has been decided not to take the SEM/AVS (SEM = simultaneously extracted metals, AVS = acid volatile sulphide) concept into account in standard-setting for metals.

3.2.1.2 MPC derivation using species sensitivity distributions

- The FHI document gives the following guidance on the ERL derivation for sediment with the SSD method: 'For sediment, long-term NOECs of 10 species representing different living and feeding conditions may be considered appropriate.' (Footnote 11, page 27).
  For metals this is explicitly mentioned (FHI [section 4.4.2.2, p. 41]): 'If sufficient NOEC data for benthic organisms are available (≥ 10 NOEC data for different species representing different living and feeding conditions) the same statistical extrapolation methodology as described in section 4.4.2 for the $MPA_{water, eco}$ is used to derive the $MPA_{sediment}$. In principle, the same methods as proposed for the derivation of sediment quality standards for organic substances may be used to derive the $MPA_{sediment}$ of metals.' Therefore, 10 chronic data for different species with different living and feeding conditions must be considered as a minimum. Such a data set should, in general, comprise crustaceans, insects and annelids, but data on benthic molluscs, echinoderms and bacteria are sometimes available as well. To date, hardly any substance has been investigated (for ERL derivation) for which the data set on toxicity data for benthic organisms was so extensive that statistical extrapolation had to be considered.
- The FHI document gives no additional information on the interpretation on micro- or mesocosm studies for the sediment compartment. If possible, an $MPC_{sediment}$ should be based on information from these studies as well.
- Finally, a comparison of the two, possibly three values from assessment factors, statistical extrapolation and field/mesocosm studies, should lead to the final choice of the MPC based on expert judgement with justification of the choices made.

3.2.2 $MPC_{marine\ sediment}$ – transitional, coastal and territorial waters

$MPC_{marine\ sediment}$ derivation for transitional, marine and coastal waters is performed according to TGD [section 4.3.2], which is also cited by FHI [p. 23, Table 6]. This approach is the same as for freshwater sediment, outlined in section 3.2.1 of this report. However, a different assessment factor scheme applies, as shown in Table 23.

FHI and TGD citation:

Table 23. Assessment factors for derivation of the $MPC_{marine,\ sediment}$ based on the lowest available EC50 from short-term tests or NOEC or EC10 from long-term tests.

Available test result	Assessment factor[a]
One acute freshwater or marine test (L(E)C50)	10000[b]
Two acute tests including a minimum of one marine test with an organism of a sensitive taxa (lowest L(E)C50)	1000[b]
One long term freshwater sediment test	1000
Two long term freshwater sediment tests with species representing different living and feeding conditions	500
One long term freshwater and one saltwater sediment test representing different living and feeding conditions	100
Three long term sediment tests with species representing different living and feeding conditions	50
Three long term tests with species representing different living and feeding conditions including a minimum of two tests with marine species	10

Notes

a. The general principles of notes (c) and (d) (TGD [section 3.3.1.1., p. 100-102, table 16]; see section 3.1.2.2 of this document) as applied to data on aquatic organisms shall also apply to sediment data. Additionally, where there is convincing evidence that the sensitivity of marine organisms is adequately covered by that available from freshwater species, the assessment factors used for freshwater sediment data may be applied. Such evidence may include data from long-term testing of freshwater and marine aquatic organisms, and must include data on specific marine taxa.

b. If an $MPC_{marine\ sediment}$ is calculated with short-term toxicity data an alternative MPC must be calculated using the equilibrium partitioning approach (see section 4.3.2.3 of the FHI; see section 3.7 of this document). The final MPC is set based on expert judgement, taking all available information into account.

End of citation

It is realised that not all possible combinations of available freshwater and marine tests are presented in the guidance from FHI presented above. Additional guidance is given below.

- We propose to use an assessment factor of 500 if only one long-term marine but no freshwater test is available.
- If two long-term tests with marine species representing different living and feeding conditions are available and no freshwater tests, an assessment factor of 100 is proposed.
- Furthermore, it is not specified what sensitive taxa are. From the table it can be deduced that an assessment factor of 1000 might only be applied to a short-term toxicity test if the lowest value available is a value for a marine species.
- If there are no sediment toxicity data for marine species and the $MPC_{sediment}$ for freshwater has been calculated using EqP, we propose that $MPC_{marine,\ sediment}$ is calculated from $MPC_{eco,\ marine}$ using EqP. For the marine environment, the extra assessment factor of 10 for the contribution of food ingestion on the value calculated by equilibrium partitioning is applied as well for substances with a log K_{ow} higher than 5.
- For the freshwater compartment it is stated that risk limits should be considered as indicative in the case of less than three chronic toxicity data, with sediment organisms representing different life and feeding conditions. Such guidance is not presented for the marine environment. It is proposed to use the same assignment for the $MPC_{marine,\ sediment}$ if there are less than three long-

term NOECs or EC10 (freshwater or marine) representing different living and feeding conditions.

- If a species sensitivity distribution is used to derive the $MPC_{sediment}$ for freshwater, this could form the basis for the $MPC_{marine\ sediment}$ as well. The same methodology as used for the preliminary effect assessment (use of assessment factors) is proposed:
  - $MPC_{marine\ sediment} = MPC_{sediment}$ if at least two typical marine species are represented;
  - $MPC_{marine\ sediment} = MPC_{sediment}/2$ if only one typical marine species is represented;
  - $MPC_{marine\ sediment} = MPC_{sediment}/5$ if no typical marine species are represented.

For metals, the same methodology is, in principle, used as described in this section. Similar to the freshwater compartment, a locally relevant background concentration should be used in the added risk approach in order to derive local quality standards (see section 3.6).

3.3 Soil compartment

The guidance for the derivation of the MPC_{soil} is based on the TGD. Before an MPC_{soil} can be derived, the sections on data handling (sections 2.2.4 and 2.2.6.2) for guidance on correct compilation of data tables, recalculation to standard soil and aggregation of multiple toxicity data for the same species should be considered.

3.3.1 Trigger values

The assessment of secondary poisoning for soil is triggered by several items [TGD, section 3.8.2, p. 122]:

- the compound has a log $K_{ow} \geq 3$; or
- the compound is highly adsorptive, or
- the compound belongs to a class of substances known to have a potential to accumulate in living organisms, or
- there are indications from structural features, and
- there is no mitigating property such as hydrolysis (half-life less than 12 hours).

If a potential for bioaccumulation exists according to these criteria, assess secondary poisoning for the terrestrial compartment. See section 3.3.5 for more detailed information.

3.3.2 Soil microbial processes and enzymatic reactions

For toxicity data on soil microbial processes and enzymatic reactions, guidance given by Traas (2001) was followed (next two sections).

Due to the nature of the endpoint, these data describe a process performed by an entire microbial community. The process is thus likely performed by more than one species. Under toxic stress, the functioning of the process may be taken over by less sensitive species. It is concluded that effects on species and effects on processes are quite different, and the results of ecotoxicological tests with microbial processes and enzymatic reactions cannot be averaged with single species tests, because of the fundamental differences between them (Van Beelen and Doelman, 1997).
For microbial and enzymatic processes, more than one value per process is included in the extrapolation method. NOECs for the same processes, but calculated from tests on different soils, are regarded as NOECs based on different populations of bacteria and/or microbes, therefore, these NOECs are treated separately. Only if values are derived from a test using the same soil, is one geometric mean value selected.

In specific cases, isolated micro organisms or fungi are used in micro tests, where they are regarded as individual species and added to the set of species NOECs.

3.3.3 Taxonomic groups and trophic levels

With regard to the classification in taxonomic groups and trophic levels for the terrestrial compartment, the following points should be regarded.

- For the purpose of ERL derivation, the TGD discerns three basic trophic levels within the terrestrial ecosystem. These are identified as primary producers (plants), consumers (e.g. invertebrates) and decomposers (e.g. micro-organisms or fungi). These levels also relate to Table 24, which shows the assessment factors when toxicity data are available for species representing these trophic levels.
- When the $MPC_{eco, soil}$ is derived using preliminary risk assessment, data on soil microbial processes and enzymatic reactions (which are collected in a separate data table) are treated as data on the trophic level of micro-organisms. The argumentation to keep these data separate is outlined in section 3.3.2. Since soil toxicity data on microbial processes and enzyme reactions are not averaged for ERL derivation (section 3.3.2), unless tested in the same soil, this means that the lowest value of all data on microbial processes and enzymatic reactions is used to represent the trophic level 'micro-organisms' in the derivation of the $MPC_{eco, soil}$. This applies both to organic compounds as well as to metals.
- When statistical extrapolation is applied to derive the $MPC_{eco, soil}$, terrestrial microbial processes and enzyme activities are treated separately from the tests on single species. Two MPCs are then derived: one for microbial processes and enzymatic reactions, and one for terrestrial species, which may include pure cultures of micro-organisms (single species tests).

3.3.4 $MPC_{eco, soil}$ – ecotoxicity in soil

The $MPC_{eco, soil}$ for organic compounds is derived according to the following scheme:

1. When no toxicity data are available for soil organisms, the equilibrium partitioning method is applied. This method is explained in section 3.7.
2. When only one test result with soil dwelling organisms is available (earthworms or plants)[28], the $MPC_{eco, soil}$ is calculated both on the basis of this result, using assessment factors given in Table 24, and by using the equilibrium partitioning method, with the $MPC_{eco, water}$ as input. The lowest value of the two is chosen as final $MPC_{eco, soil}$ value.
3. When toxicity data are available for a producer and/or a consumer and/or a decomposer, the $MPC_{eco, soil}$ is calculated using assessment factors as presented in Table 24. An $MPC_{eco, soil}$ is calculated on the basis of the lowest determined effect concentration (e.g. NOEC, EC10 or L(E)C50). It should be noted that it is not specified whether or not this effect concentration originates from a chronic or acute toxicity study.[29] If results from short-term tests with a producer and/or a consumer and/or a decomposer are available, the result is divided by a factor of 1000 to calculate the $MPC_{eco, soil}$. Although data for all three levels are preferred, a base set

[28] The mentioning of earthworms or plants in parentheses is considered as an example. The TGD does not give guidance for the case that there is only one toxicity value, but this is not an earthworm or a plant, e.g. an insect or a microbial process. Therefore the same procedure should be followed in such a case.

[29] This guidance deviates from the guidance on the aquatic PNEC. For the aquatic compartment the effect concentrations are first divided by the appropriate assessment factor, after which the lowest value is chosen as PNEC. For soil, the lowest effect concentration is first identified as basis for the PNEC and then the appropriate assessment factor is applied. In exceptional cases it may occur that the lowest EC50 from a different terrestrial trophic level is almost equal or only marginally higher than the lowest NOEC. In such a case, the choice of the right assessment factor has to rely on expert judgment. The TGD states that the assessment factors must be regarded as indicative.

similar to the aquatic environment is currently not available and is therefore not required for soil.

4. Calculation of an $MPC_{eco, soil}$ using statistical extrapolation techniques can be considered when sufficient data are available. The TGD refers in this case to the minimum requirements for the aquatic environment. However, the species mentioned are evidently not representative for the terrestrial compartment (see section 3.1.2.1 for minimum requirements for the aquatic environment). The guidance on this subject must therefore be regarded as incomplete. Similar to the aquatic compartment, the minimum data set to calculate a species sensitivity distribution should contain chronic toxicity data for at least 10 species from different taxonomic groups. For comparable data on the same endpoint and species, the geometric mean by default should be used as the input value for the calculation of the species sensitivity distribution. When results are available from tests using different soils, it is likely that the soil characteristics have an influence on the results. The effect data should be normalised before further processing (section 2.2.4.15). If not possible (e.g. for some metals), the lowest NOEC of the most sensitive endpoint for species should be used. Data on microbial-mediated processes and single-species tests should be considered separately due to fundamental differences between these tests (functional vs. structural test, multi-species vs. single species, adapted indigenous microbe community vs. laboratory test species, variability of test design and different endpoints, etc.). The results should be compared and evaluated on a case-by-case basis in deciding on a final PNEC for the soil compartment. The approach of statistical extrapolation for the soil compartment is still under debate and needs further validation.
5. Currently, no guidance is available on the performance and evaluation of model ecosystems or multi-species terrestrial field studies. However, these data should be considered in the derivation of the MPC for soil in a similar manner as for the aquatic and sediment compartment (see sections 3.1.2.4 and 3.2.1.2). Guidance for the interpretation of earthworm field studies is available and may be useful in interpretation of earthworm field studies (De Jong *et al.*, 2006).

TGD citation:

Table 24. Assessment factors for derivation of $MPC_{eco, soil}$.

Available test result	Assessment factor
L(E)C50 short-term toxicity test(s) (e.g. plants, earthworms, or micro organisms)	1000
NOEC for one long-term toxicity test (e.g. plants)	100
Two long-term NOECs from species representing two trophic levels	50
Long-term NOECs from at least three species representing three trophic levels	10
Species sensitivity distribution (SSD method)	5–1, to be fully justified on a case-by-case basis (cf. main text)
Field data/data of model ecosystems	case-by-case

Note: The text from the table is not literally copied from the TGD but for clarity it has been brought in accordance with the table with assessment factors for the aquatic compartment. Note that the footnotes under the table for the aquatic compartment (section 3.1.2.2) can not be translated directly to this table.

End of citation

For $MPC_{eco, soil}$ derivation for metals, the added risk approach (section 3.6) is followed. The $MPA_{eco, soil}$ is derived following the same procedure as described above for the MPC.

3.3.5 $MPC_{sp, soil}$ – secondary poisoning in soil

Following TGD guidance, the assessment of secondary poisoning via the terrestrial food chain is triggered by several items as described in section 3.3.1. The $MPC_{sp, soil}$ is calculated using the following procedure:

1. First, an MPC_{oral} for birds and/or mammals is derived for each experiment, in the same way as done for the route of secondary poisoning for the aquatic environment (section 2.2.7.2, Eqs. 4 to 5, section 3.1.4, Eqs. 11 and 12, and Table 21.
2. Select the *lowest* of the available MPC_{oral} values for different species for calculation of the $MPC_{sp, soil, TGD}$. If enough data are available for mammals and birds the use of statistical extrapolation can be considered. See for more detail section 3.1.4.2.
3. If no experimental bioaccumulation data for soil are available, the $MPC_{sp, soil, TGD}$ [$mg.kg_{dw}^{-1}$] is calculated using Eq. 27. In this case, the $BCF_{earthworm}$ is estimated using a QSAR (see section 2.3.4.2). This equation is based on dry weight of the soil:

$$MPC_{sp,soil,TGD} = \frac{MPC_{oral,min} \cdot (1 + F_{gut} \cdot CONV_{soil})}{BCF_{earthworm} \cdot \frac{RHO_{soil}}{K_{soil-water} \cdot CONV_{soil} \cdot 1000} + F_{gut}} \quad (27)$$

$$CONV_{soil} = \frac{RHO_{soil}}{Fsolid_{soil} \cdot RHO_{solid}} \quad (28)$$

- Eq. 27 is derived from the TGD [TGD Eq. 82c, page 132]. The original equation contains both a concentration in pore water and in soil, expressed on wet weight basis. The relationship between the concentration in pore water and the concentration in soil is described at page 85 of the TGD [TGD Eq. 67]. TGD Eq. 67 was substituted in 82c and rewritten to give Eq. 27.
- $K_{soil-water}$ should be calculated using Eq. 59 together with Eqs. 57 and 60 for organic chemicals, with comp = soil, and the appropriate values from sections 2.1.3.2 for the K_{oc}, 2.1.3.6 for Henry's law constant of organic chemicals, and 2.1.2.6 for the K_p of metals.
- The calculation is preferably based on experimental bioaccumulation studies with earthworms (see section 2.3.4.1). The results from such studies are expressed as the ratio between the concentration in worms based on wet weight and the concentration in soil based on dry weight, preferably normalised to the standard soil of the TGD. The $MPC_{sp, soil, TGD}$ is then calculated by the following equation:

$$MPC_{sp,\ soil,TGD} = \frac{MPC_{oral,min} \cdot (1 + F_{gut} \cdot CONV_{soil})}{BSAF_{earthworm} + F_{gut}} \quad (29)$$

- The calculated $MPC_{sp, soil, TGD}$ should be normalised to Dutch standard soil by the procedure described in section 3.7.4. This conversion finally gives the $MPC_{sp, soil}$.

3.3.6 $MPC_{human, soil}$ – human-toxicological risk limits for soil

On the Dutch national scale, human-toxicological environmental risk limits ($MPC_{human, comp}$) have to be derived for all environmental compartments; the national guidance (this report) is used for derivation of $MPC_{human, soil}$. For explanation on the background of the $MPC_{human, comp}$, see section 1.5.

The model HUMANEX (Bontje *et al.*, 2005) was tested for the purpose of calculating $MPC_{human, comp}$ values. HUMANEX uses the steady state multi-compartment model Simplebox as an integrated part of EUSES 2.0. However, use of HUMANEX was deemed undesirable for the derivation of generic environmental risk limits based on human health. The following explains this decision. Calculating a steady-state distribution of a compound over the various environmental compartments means that changing the concentration in one compartment directly influences the concentrations in

all the other compartments. When a compound is highly toxic to humans and enters the human body primarily via one route (e.g. a volatile compound via air), this would result in a very low $MPC_{human, air}$. Due to the assumption of steady-state between the compartments, the concentrations in the other compartments would be lowered accordingly, resulting in very low $MPC_{human, comp}$ values for those compartments. For the example of a volatile toxic compound, the resulting environmental standards in soil would be very low, while the compound does not pose a problem in soil. This problem is less prominent for compounds that are more evenly distributed over the environmental compartments (i.e. when the assumption of steady-state between homogeneous compartments becomes more realistic).

The WFD-FHI strategy employed for the water compartment is chosen as a pragmatic approach. Specific human intake routes are allowed to contribute 10% of the human toxicological threshold limit (e.g. TDI). The intake routes are based on compartment concentrations that are not in steady-state equilibrium. For the water compartment, the routes of fish consumption and drinking-water consumption have already been defined. Four uptake routes of human exposure that are related to a concentration in soil and groundwater are defined in the modelling approach from EUSES. The models put forward in FHI guidance for water are also in line with the EUSES model.

The equations in the following sections were taken from the EUSES 2.0 manual (European Commission, 2004a) and rewritten in order to calculate $MPC_{human, soil}$ values. Four different routes contributing to human exposure have been incorporated: consumption of leafy crops, root crops, milk and meat. First the concentration in the leaf, root, milk or meat is calculated as a 10% fraction of the TDI, taking into account the daily dietary intake of these products. The concentration in leaf, root, milk and meat are then each recalculated to a concentration in soil: $MPC_{human, soil, leaf}$, $MPC_{human, soil, root}$, $MPC_{human, soil, milk}$ and $MPC_{human, soil, meat}$. The lowest of the four values is selected and is the final $MPC_{human, soil}$.

Average dietary intake rates of the various components (IH_{leaf}, IH_{root}, IH_{milk}, IH_{meat} in $kg_{ww}.d^{-1}$) were also selected from EUSES 2.0; values for these and other defaults as well as all the description of all variables can be found in Table 31.

3.3.6.1 Exposure via consumption of leaf crops

First, a 10% fraction ($F_{TDI, leaf}$) of the TDI is expressed as a concentration in leaf:

$$C_{leaf} = \frac{F_{TDI,\ leaf} \cdot TDI \cdot BW}{IH_{leaf}} \qquad (30)$$

The following equations from EUSES are needed; some are rearranged (Eq. 31 to 37):

$$K_{plant-water} = Fwater_{plant} + Flipid_{plant} \cdot K_{ow} \qquad (31)$$

$$K_{leaf-air} = F\mathrm{air}_{plant} + \frac{K_{plant\text{-}water}}{K_{air\text{-}water}} \qquad (32)$$

$$kelim_{plant} = kmetab_{plant} + kphoto_{plant} \qquad (33)$$

$$ALPHA = \frac{AREA_{plant} \cdot g_{plant}}{K_{leaf-air} \cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant} \qquad (34)$$

C_{leaf} from Eq. 30 is entered in Eq. 35:

$$BETA_{agric} = C_{leaf} \cdot RHO_{plant} \cdot ALPHA \qquad (35)$$

$$TSCF = 0.784 \cdot \exp\left[\frac{-(\log K_{ow} - 1.78)^2}{2.44}\right] \qquad (36)$$

$$C_{agric,porew,\ leaf} = \frac{BETA_{agric}}{TSCF \cdot \frac{Q\text{transp}}{V_{leaf}} + (1 - F\text{ass}_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}} \qquad (37)$$

C_{air} is set to zero.

- The resulting $C_{agric,\ porew,\ leaf}$ is recalculated to a concentration in soil, C_{soil}, using Eq. 38, for which Eq. 57 through Eq. 60 are needed, with comp = soil.

$$C_{soil} = \frac{C_{agric,\ porew,\ leaf} \cdot K_{soil-water}}{RHO\text{soil}} \qquad (38)$$

- The resulting value is expressed in wet weight soil, which is recalculated to dry weight soil using Eq. 64.
- Finally, the value expressed in dry weight is recalculated to Dutch standard soil (dry weight), using Eq. 65 to obtain the $MPC_{human,\ soil,\ leaf}$.

3.3.6.2 Exposure via consumption of root crops

First, a 10% fraction of the TDI is expressed as a concentration in root:

$$C_{root} = \frac{F_{TDI,\ root} \cdot TDI \cdot BW}{IH_{root}} \qquad (39)$$

The following (rearranged) equation from EUSES is needed:

$$C_{agric,porew,\ root} = \frac{C_{root} \cdot RHO_{plant}}{K_{plant-water}} \qquad (40)$$

- $C_{agric,\ porew,\ root}$ is the pore water concentration. The corresponding concentration in soil is calculated using Eq. 38, by replacing $C_{agric,\ porew,\ leaf}$ with $C_{agric,\ porew,\ root}$.
- The resulting value is expressed in wet weight soil. The MPC is recalculated to dry weight soil using Eq. 64.
- Finally, the value expressed in dry weight is recalculated to Dutch standard soil (dry weight), using Eq. 65 to obtain the $MPC_{human,\ soil,\ root}$.

3.3.6.3 Exposure via consumption of milk

First, a 10% fraction of the TDI is expressed as a concentration in milk:

$$C_{\text{milk}} = \frac{F_{\text{TDI, milk}} \cdot TDI \cdot BW}{IH_{\text{milk}}} \quad (41)$$

The following equations from EUSES are needed (Eq. 42 to 45):

$$BAF_{\text{milk}} = 10^{-8.1+\log K_{\text{ow}}} \quad (42)$$

$$IC_{\text{grass}} = ICdwt_{\text{grass}} \cdot CONV_{\text{grass}} \quad (43)$$

$$IC_{\text{soil}} = ICdwt_{\text{soil}} \cdot CONV_{\text{soil}} \quad (44)$$

$$C_{\text{milk}} = BAF_{\text{milk}} \cdot C_{\text{grass}} \cdot IC_{\text{grass}} + BAF_{\text{milk}} \cdot C_{\text{grassland}} \cdot IC_{\text{soil}} \quad (45)$$

In comparison with the original equation in EUSES, the concentrations in air and drinking water are set at zero. The contribution of this drinking-water uptake route is negligible compared to direct drinking-water uptake of 2 L incorporated in the $MPC_{\text{dw, water}}$. Both the concentration in grass (C_{grass}) and grassland soil ($C_{\text{grassland}}$) are needed, since cattle eat both grass and ingest soil. C_{grass}, calculated by Eq. 46, is in equilibrium with $C_{\text{grassland}}$ since C_{grass} is dependent on $C_{\text{grassland, porew}}$ (see Eq. 47), i.e. the pore water concentration in the soil beneath the grassland.

$$C_{\text{grass}} = \frac{BETA_{\text{grass}}}{ALPHA} \cdot \frac{1}{RHO_{\text{plant}}} \quad (46)$$

$$BETA_{\text{grass}} = C_{\text{grassland, porew}} \cdot TSCF \cdot \frac{Q\text{transp}}{V_{\text{leaf}}} + (1 - F\text{ass}_{\text{aer}}) \cdot C_{\text{air}} \cdot g_{\text{plant}} \cdot \frac{AREA_{\text{PLANT}}}{V_{\text{leaf}}} \quad (47)$$

$C_{\text{grassland, porew}}$ is substituted by its corresponding concentration in soil, $C_{\text{grassland}}$, via Eq. 38 in which $C_{\text{agric, porew, leaf}}$ is replaced by $C_{\text{grassland, porew}}$. In calculations, C_{air} is set at zero. Eq. 47 is then transformed to a simplified form:

$$BETA_{grass} = C_{\text{grassland}} . Q \quad (48)$$

with

$$Q = \frac{RHO_{\text{soil}}}{K_{soil-water}} \cdot TSCF \cdot \frac{Q\text{transp}}{V_{\text{leaf}}} \quad (49)$$

Substituting Eq. 48 into 46, results in an expression of $C_{\text{grassland}}$ in C_{grass}:

$$C_{\text{grass}} = C_{\text{grassland}} \cdot \frac{Q}{ALPHA \cdot RHO_{\text{plant}}} \quad (50)$$

Combining Eq. 45 and Eq. 50 and rearranging, gives:

$$C_{\text{grassland}} = \frac{C_{milk}}{BAF_{\text{milk}} \cdot (\frac{Q}{ALPHA \cdot RHO_{plant}} \cdot IC_{\text{grass}} + IC_{\text{soil}})} \quad (51)$$

- $C_{\text{grassland}}$ is expressed in wet weight soil. This value is recalculated to dry weight soil by Eq. 64.
- Finally, the value expressed in dry weight is recalculated to Dutch standard soil (dry weight) using Eq. 65, to obtain the $MPC_{\text{human, soil, milk}}$.

3.3.6.4 Exposure via consumption of meat

First, a 10% fraction of the TDI is expressed as a concentration in meat:

$$C_{\text{meat}} = \frac{F_{\text{TDI, meat}} \cdot TDI \cdot BW}{IH_{\text{meat}}} \quad (52)$$

The following EUSES equations are needed (Eq. 53 and 54 plus Eq. 43 and 44):

$$C_{\text{meat}} = BAF_{\text{meat}} \cdot C_{\text{grass}} \cdot IC_{\text{grass}} + BAF_{\text{meat}} \cdot C_{\text{grassland}} \cdot IC_{\text{soil}} \quad (53)$$

$$BAF_{\text{meat}} = 10^{-7.6+\log K_{\text{ow}}} \quad (54)$$

In comparison with the original equation of Eq. 53 in EUSES, the concentrations in air and drinking water are set at zero. In this case too, the contribution of this drinking-water uptake route is negligible compared to direct drinking-water uptake of 2 L incorporated in the $MPC_{\text{dw, water}}$.
The routine described for the concentration in milk (previous section), in equations 46 through 50 also apply to this route. This gives the following equation for the concentration in soil:

$$C_{\text{grassland}} = \frac{C_{meat}}{BAF_{\text{meat}} \cdot (\frac{Q}{ALPHA \cdot RHO_{plant}} \cdot IC_{\text{grass}} + IC_{\text{soil}})} \quad (55)$$

- $C_{\text{grassland}}$ is expressed in wet weight soil. This value is recalculated to dry weight soil by Eq. 64.
- Finally, this value expressed in dry weight is recalculated to Dutch standard soil (dry weight) using Eq. 65, to obtain $MPC_{\text{human, soil, meat}}$.

3.3.7 Selection of the final MPC for the soil compartment

A series of MPC values for the soil compartment has now been derived. The number of MPC values available depends on the characteristics of the compound and on data availability. The following MPC_{soil} values can potentially be derived:

$MPC_{\text{eco, soil}}$	MPC_{soil} based on ecotoxicological data
$MPC_{\text{sp, soil}}$	MPC_{soil} based on secondary poisoning
$MPC_{\text{human, soil, leaf}}$	MPC_{soil} based on human consumption of leaf crops
$MPC_{\text{human, soil, root}}$	MPC_{soil} based on human consumption of root crops
$MPC_{\text{human, soil, milk}}$	MPC_{soil} based on human consumption of milk crops
$MPC_{\text{human, soil, meat}}$	MPC_{soil} based on human consumption of meat crops

The final value for the MPC_{soil} is the lowest of the available MPC values.

3.4 Groundwater compartment

3.4.1 ERL derivation

3.4.1.1 $MPC_{eco, gw}$ – ecotoxicity for groundwater

Within the project INS, ecotoxicological ERLs for the groundwater compartment are derived based on ecotoxicological data for the surface-water compartment ($MPC_{eco, water}$, $SRC_{eco, water}$). Data on the toxicity of compounds to groundwater-inhabiting organisms are scarce. Micro-organisms (bacteria, actinomycetes, fungi, algae and protists) are the dominant life form in the subsurface. Of the multicellular organisms that have adapted to subsurface conditions, invertebrate species (Crustacea) form the majority, but species including Acari, Nematoda, Gastropoda have also been identified (Notenboom *et al.*, 1999). It is relatively difficult to collect representative organisms since, generally, the groundwater compartment is not easily accessible. Moreover, higher organisms that are known to inhabit groundwater are difficult to rear in the laboratory. Therefore, tests can only be performed with field collected animals (Notenboom *et al.*, 1999). Since groundwater-specific ecotoxicological information is virtually absent, the derived ERLs for surface water based on ecotoxicological data, are taken as substitute.

3.4.1.2 $MPC_{human, gw}$ – human-toxicological risk limit for groundwater

Further, the abstraction of groundwater for use in drinking-water preparation is important. For this purpose groundwater has to meet the same quality requirements as surface water:
the $MPC_{human, gw}$ is equal to $MPC_{dw, water}$.

At the time of writing, the methodology for the setting of threshold values for groundwater under the WFD was not fully clear. If future regulations may come into effect, which lead to human toxicological risk limits for groundwater that are lower than currently laid down for drinking water prepared from surface water, the selection of $MPC_{human, gw}$ may need to be revised.

3.4.1.3 Selection of the final MPC for the groundwater compartment

The following MPC_{gw} values can potentially be derived:

- $MPC_{eco, gw}$, which is the MPC_{gw} based on ecotoxicological data;
- $MPC_{human, gw}$, which is the MPC_{gw} for drinking-water abstraction.

The final value for the MPC_{gw} is the lowest of the available MPC values.

3.4.2 Use of dissolved versus total standards for groundwater

An important difference between FHI guidance and former INS methodology is that now (under FHI guidance) an environmental standard based on the outcome of ecotoxicological laboratory experiments (e.g. the $MPC_{eco, water}$) is considered to be **total** concentration. 'Total' in this respect, means that this concentration consists of a dissolved concentration + a concentration adsorbed to suspended particulate matter. This total concentration is thought to directly reflect the surface water in the field situation, containing e.g. 15 $mg.L^{-1}$ suspended matter (EU standard).

This differs fundamentally from former INS methodology, where standards based on ecotoxicological data were thought to reflect a dissolved concentration. A total concentration could be derived, if this was desired, by calculating a concentration adsorbed to suspended matter and adding this to the dissolved fraction. In former INS methodology, the standards for groundwater were set equal to the standards expressed as a dissolved concentration: i.e. based on the laboratory

data, since the amount of suspended matter in groundwater is considered to be much lower than that in surface water.
Since it is preferred in the INS framework to keep groundwater standards equal to standards based on the outcome of ecotoxicological studies, the $MPC_{eco, water}$ and the $SRC_{eco, water}$ (as derived according to sections 3.1.2 and 4.3) will be used to this end. Note that this is equal to the former INS procedure.

3.4.3 Relation of Dutch ERLs to EU groundwater threshold values

The concept EU Groundwater Directive defines 'threshold values' for groundwater as groundwater quality criteria which have to be set by EU member states. Upon implementation of the Groundwater Directive, the Netherlands will have the obligation to derive threshold values. In their advice to the State Secretary of the Ministry of Housing, Spatial Planning and the Environment, the Dutch Technical Committee on Soil Protection (TCB) expresses the opinion that either the target value (the environmental quality objective that is based on the NC) or the MPC would be suitable standards to serve as groundwater threshold values (Technische commissie bodembescherming, 2005).

3.5 Air compartment

3.5.1 $MPC_{eco, air}$ – ecotoxicity via air

No national guidance has been laid down for derivation of ecotoxicological environmental risk limits for the compartment air. Recently, De Jong *et al*. have derived ERLs for several volatile aliphatic hydrocarbons (De Jong *et al.*, 2007). It is proposed to follow the methodology as followed (and reported) in De Jong *et al*. for derivation of the $MPC_{eco, air}$.

3.5.2 $MPC_{human, air}$ - human toxicological risk limit for air

Human exposure via air is covered via the Tolerable Concentration in Air (TCA). The TCA is an existing standard ($\mu g.m^{-3}$) aimed at protection of humans from deleterious effects after continuous lifetime exposure via air. If a TCA is not available for the substance investigated, the databases mentioned in section 2.4.1 may be searched for risk limits in air that can be used for this purpose. In principle, the RfC (reference concentration), derived by the U.S. EPA can be considered useful. Be aware that an RfC is always based on non-cancer effects and this standard may not be protective for carcinogenic substances. Consult an expert in human toxicology to verify the usefulness of the retrieved risk limit(s).

3.5.3 Selection of the final MPC for the air compartment

The following MPC_{air} values can potentially be derived:

- $MPC_{eco, air}$, which is the MPC_{air} based on ecotoxicological data;
- $MPC_{human, air}$, which is the MPC_{air} based on chronic inhalation.

The final value for the MPC_{air} is the lowest of the available MPC values.

3.6 Environmental risk limits for metals

For derivation of ERLs for metals, FHI proposes to follow the added risk approach as used and described by e.g. Crommentuijn *et al*. (1997). The FHI guidance also notes that the recent developments in the area of biotic ligand models (BLM) may be used in the future for the assessment of bioavailability and the calculation of local quality standards after comprehensive data have become available for validation. However, up to now the added risk approach is considered preferable because of its merits for setting regulatory standards. The following sections, cited from Traas (2001) with slight modifications, introduce this method.

The added risk approach, which is modified from Struijs *et al*. (1997), is used to take natural background concentrations into account when calculating MPCs for naturally occurring substances. The approach starts by calculating a maximum permissible addition (MPA) on the basis of available data from laboratory toxicity tests (with added amounts of toxicants). This MPA is considered to be the maximum concentration to be added to the background concentration (C_b), without causing deleterious effects. Hence, the MPC is the sum of C_b and MPA:

$$MPC = C_b + MPA \qquad (56)$$

The background concentration and the MPA are independently derived values. The MPA is calculated using a similar approach as the MPC for substances having no natural background concentration (see sections 3.1.2 to 3.1.5 for water and sections 3.2 for sediment and 3.3 for soil), except for drinking water. The MPC for drinking water is always based on total concentrations in water and the added risk approach is not applied (section 3.1.6). The background concentration is thus always part of the ERL and therefore the ERL cannot approach zero. The implicit assumption is that the background concentration has resulted in the biodiversity of ecosystems or serves to fulfil the need for micronutrients of species in the environment (Klepper *et al.*, 1998).

With regard to the bioavailable fraction of the metals in laboratory tests, we assume that the metals that are added to the test medium are fully bioavailable, i.e. the bioavailable fraction of the added metal in laboratory tests is 100%. The theoretical description of the added risk approach, as described by Struijs *et al*. (1997), includes a further refinement by allowing the bioavailable fraction of the background concentrations to vary between 0% and 100% (Crommentuijn *et al.*, 2000). However, to which extent the metals are bioavailable is not relevant, since any potential adverse or positive effect of metals originating from the background is considered not to be deleterious because of its contribution to biodiversity. Besides that, at the moment there is insufficient information available to derive the bioavailability of the background concentrations for metals. When bioavailability is theoretically varied, the resulting MPCs do not differ greatly from the MPC with bioavailability set at 0% (Crommentuijn *et al.*, 2000). In conclusion, in ERL derivation within the INS framework, the fraction of the background concentration that is bioavailable is set at zero for metals.

3.7 Equilibrium partitioning method

Here, the equilibrium partitioning (EqP) method is explained. The procedure outlined is identical to the guidance given in the TGD, for the suspended matter, soil and sediment compartments. The FHI guidance cites the TGD on this subject. However, because Dutch standard soil, sediment and

suspended matter have different values for the organic matter content, a recalculation to Dutch standard soil, sediment and suspended matter is included as an additional step in the EqP method.

3.7.1 Calculation of $K_{comp\text{-}water}$

In the EqP method outlined in the TGD, the 'dimensionless' partition coefficient $K_{comp\text{-}water}$ is used, in units of $m^3.m^{-3}$. This parameter is also called the total compartment-water partition coefficient. It is calculated, for each compartment of interest according to the equations given on p. 47 (part II) of the TGD. Note that EqP to the bulk-sediment compartment is not performed within the current guidance (see 3.7.2), although the parameters for its calculation are given below for reasons of completeness.

$$Kp_{comp} = Foc_{comp} \times K_{oc} \quad with\ comp \in \{ soil, sed, susp \} \tag{57}$$

$$K_{comp-water} = \frac{Ctotal_{comp}}{Cporew_{comp}} \tag{58}$$

$$K_{comp-water} = Fair_{comp} \times K_{air-water} + Fwater_{comp} + Fsolid_{comp} \times \frac{Kp_{comp}}{1000} \times RHOsolid \tag{59}$$

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

$$K_{air-water} = \frac{H}{R} \times TEMP \tag{60}$$

The default values for compartment-specific characteristics ($Fair_{comp}$, RHOsolid, etc.) from the TGD [section 2.3.4, p. 44] should be used in these equations; their values are listed in the list variables and default values (Table 31).

3.7.2 EqP for sediment

Please note that, *following TGD and FHI guidance*, the characteristics of suspended matter are used in EqP calculations for sediment rather than the characteristics of bulk-sediment. This is done since the derived $MPC_{sediment}$ should reflect the concentration in the upper layer of the sediment rather than the concentration in the bulk sediment. The rationale behind the choice for an ERL for the upper sediment layer is that the major part of exposure for sediment dwelling organisms is thought to occur via the upper part of the sediment rather than via the deeper sediment layers. Bioavailability of the substance adsorbed to suspended matter is believed to be higher. Nevertheless, there is no methodological difference behind this choice for suspended matter, because in both cases the equilibrium partitioning method is used. Moreover, due to the higher organic matter content of suspended matter in comparison to sediment in the default values of the TGD (see section 1.6 of this report), the values based on dry weight are higher. For this reason, an inconsistency is introduced with the direct toxicity data for benthic organisms, which are normalised to the organic matter content of sediment (see section 2.2.4.15). However, by recalculation to Dutch standard sediment from suspended matter (see section 3.7.4), this problem is largely circumvented.

The calculation of the MPC for sediment by equilibrium partitioning according to the TGD and FHI is given below.

- The $MPC_{sediment, EqP, dw}$ is calculated according to EqP from the MPC for aquatic organisms, $MPC_{eco, water}$, using Eqs. 61 and 62, or in the case of marine sediment, from $MPC_{eco, marine}$.
- When the $MPC_{sediment}$ has been calculated using EqP and log $K_{ow} > 5$ for the compound of interest, $MPC_{sediment}$ is divided by 10. This correction factor is applied because EqP only considers uptake via the water phase. Extra uncertainty due to uptake by ingestion of food should be covered by the applied assessment factor of 10.
- It should be noted that in the case of metals, only empirically derived values for $K_{susp\text{-}water}$ should be derived [FHI footnote 27, p. 41].

$$MPC_{sediment, TGD, EqP, ww} = \frac{K_{susp-water}}{RHO_{susp}} \times MPC_{eco, water} \times 1000 \quad (61)$$

$$MPC_{sediment, TGD, EqP, dw} = \frac{RHO_{susp}}{Fsolid_{susp} \times RHOsolid} \times MPC_{sediment, TGD, EqP, ww} \quad (62)$$

The default values for suspended matter characteristics ($Fsolid_{susp}$, RHO_{susp}, etc.) have been taken from the TGD [section 2.3.4, p. 44]; these are listed in Table 31. The formulae, parameters and default characteristics necessary to calculate the density are also mentioned in section 2.3.4 of the TGD and will not be repeated here.

3.7.3 EqP for soil

The calculation of the MPC_{soil} in the TGD by equilibrium partitioning follows the same route as for sediment:

- The MPC_{soil} is calculated according to EqP from the MPC for aquatic organisms, $MPC_{eco, water}$, using Equation 63.
- When the MPC_{soil} is calculated using EqP and log $K_{ow} > 5$ for the compound of interest, MPC_{soil} is divided by 10. This correction factor is applied because EqP only considers uptake via the water phase. Extra uncertainty due to uptake by ingestion of food should be covered by the applied assessment factor of 10.

$$MPC_{soil, TGD, EqP, ww} = \frac{K_{soil-water}}{RHO_{soil}} \times MPC_{eco, water} \times 1000 \quad (63)$$

$$MPC_{soil, TGD, EqP, dw} = \frac{RHO_{soil}}{Fsolid_{soil} \times RHOsolid} \times MPC_{soil, TGD, EqP, ww} \quad (64)$$

The values for the environmental compartment characteristics (*viz*. $Fsolid_{soil}$ and RHO_{soil}) have been taken from the TGD [section 2.3.4, p. 43]; these are listed in Table 31. The formulae, parameters and default characteristics necessary to calculate the density are also mentioned in section 2.3.4 of the TGD and will not be repeated here.

3.7.4 Recalculation to Dutch standard soil and sediment

The resulting values are numbers for sediment and soil with the characteristics of suspended matter and soil according to the TGD. These values should be recalculated to Dutch standard sediment and

soil. Both standard sediment and soil contain 10% organic matter, which is equivalent to 5.88% organic carbon (calculated using Eq. 2):

$$MPC_{\text{Dutch standard sediment/soil, EqP, dw}} = \frac{Foc_{\text{Dutch standard sediment/soil}}}{Foc_{\text{susp/soil, TGD}}} \times MPC_{\text{sediment / soil, TGD EqP, dw}} \quad (65)$$

The values of the parameters are listed in section 1.6.

The resulting values for standard sediment are different from those obtained by the method presented in Janssen *et al.* (2004). In that report, the *F*oc of sediment from the TGD was used in Equation 65 instead of the *F*oc of suspended matter, while for the rest, all parameters of suspended matter were been adapted. This results in a concentration in Dutch standard sediment that is twice as high. As an illustration, results of the different calculation methods using two combinations of (fictitious) MPC and log K_{oc} are shown in Table 25.

The differences between standard soil, sediment, and sediment with suspended matter characteristics are caused by the differences in the fraction water of the compartment, since the fraction organic matter of Dutch standard soil and sediment is the same. As can be seen from Table 25, for hydrophobic substances (log K_p = 6) –which are fully associated with the solid phase– the calculated MPC for a soil or sediment with 10% organic matter (Dutch standard soil or sediment) is the same regardless of the chosen characteristics. For these compounds it is evident that the recalculation as proposed in Janssen *et al.* (2004) is incorrect.

It is realised that this normalisation from concentrations based on dry weight as defined in the TGD to dry weight in Dutch standard soil and sediment is theoretically not correct, because it is assumed that the total concentration can be normalised to organic carbon. In reality, only the fraction of compound associated with the solid part of the sediment can be normalised to organic carbon, not the fraction of compound present in the water fraction of sediment. As can be seen from Table 25, the differences between normalised values for suspended matter and sediment according to the TGD are relatively small, even for non-hydrophobic substances. This is due to the almost equal ratio between water and organic carbon in sediment and suspended matter. However, this does not hold for sediment and suspended matter with the organic carbon content of Dutch standard sediment. When applying equations 61 and 62 directly with the organic carbon content of Dutch standards, the resulting value for sediment is 21.88 $mg.kg_{dw}^{-1}$ with sediment characteristics, and 41.88 $mg.kg_{dw}^{-1}$ with suspended matter characteristics. The proposed EqP method thus yields correct values for sediments in which the ratio of organic carbon content to the fraction water is around the value that comes from the defaults as defined in the TGD.

Table 25: MPCs for standard soil or sediment obtained with different methods to normalise concentrations to organic matter. Results obtained using two combinations of MPC and log K_{oc}, both fictitious.

Substance	$MPC_{sediment}$ from TGD suspended matter characteristics	$MPC_{sediment}$ from TGD sediment characteristics	$MPC_{sediment}$ according to Janssen *et al*. 2004	MPC_{soil} from TGD soil characteristics	MPC from *K*p (old INS method for soil and sediment)
MPC=10 $mg.L^{-1}$, log K_{oc}=1.00	27.06	24.71	54.12	9.81	5.88
MPC=0.0001 $mg.L^{-1}$, log K_{oc}=6.00	5.88	5.88	11.77	5.88	5.88

4. Derivation of MAC, NC and SRC_{eco}

4.1 $MAC_{eco, water}$ – intermittent release/short-term exposure

MAC stands for maximum acceptable concentration. The MAC is intended to protect the *aquatic* ecosystem 'against acute toxic effects exerted by exposure to short-term peak concentrations' or 'against acute effects of transient exposure peaks' (citations FHI). The $MAC_{eco, water}$, introduced by the WFD, is an ERL that is new to the Dutch framework of standard-setting. According to the FHI guidance it is appropriate to derive a MAC_{eco} for water only, because in other compartments such as sediment and biota, the changes in concentrations are much slower. A peak concentration as may be observed for water will not be relevant for these compartments.

Guidance for derivation of the $MAC_{eco, water}$ (using assessment factors) is cited in the next section. This guidance is taken from the FHI [section 4.3.6], which, in turn, is partly based on TGD guidance for substances with 'intermittent release' [TGD, section 3.3.2]. FHI adds the possibility of basing the $MAC_{eco, water}$ on a species sensitivity distribution for acute toxicity data and on the results of micro/mesocosm studies. The three possibilities will be discussed below. The choice for the final $MAC_{eco, water}$ value should be explained in a comparison of the different methods. See also section for extra guidance on the selection of the final MAC value.

MAC_{eco} for freshwater and marine water
Although not explicitly mentioned in FHI guidance, a MAC_{eco} may also be derived for the marine compartment, if this is desired from a regulatory point of view. Derivation of a $MAC_{eco, marine}$ should be considered on a case by case basis, depending on the substance investigated and taking toxicological considerations (e.g. sensitivity of freshwater versus marine species) into account.

4.1.1 Derivation of $MAC_{eco, water}$ based on assessment factors

FHI citation, p. 37.
For exposure of short duration only short-term effects may need to be considered. An assessment factor of 100, applied to the lowest L(E)C50 of at least three short-term tests of three trophic levels, is normally considered appropriate to derive the MAC-QS for such situations. However, 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, interspecies variations may be low and therefore a factor lower than 100 appropriate. Expert judgement and justification of the decision regarding the assessment factor chosen is therefore required. In no case should a factor lower than 10 be applied to a short-term L(E)C50 value. (TGD)
End of citation.

Additional INS guidance
- When a $MAC_{eco, water}$ is to be derived, the above guidance from the TGD ('intermittent release') and FHI can be used. However, since the guidance is very brief, the FHI guidance is translated into a decision table (Table 26), including additional information which is indispensable to determine the choice of the assessment factors.
- The $MAC_{eco, water}$ is derived using the toxicity data tabulated in the aggregated data table, as described in section 2.2.6.1. This means that the $MAC_{eco, water}$ is based on all available acute toxicity data for aquatic species, on both lethal and/or sublethal endpoints. More detail on

toxicity is provided in the toxicity data table, which shows all individual tests (this table is described in detail in section 2.2.3).

- FHI and TGD guidance do not quantify 'potential to bioaccumulate' in their sections on $MAC_{eco, water}$ derivation. However, FHI does explicitly trigger secondary poisoning with an experimental BCF $\geq$ 100 or BMF > 1 (both are defined without units) and in case of absence of both, a log $K_{ow} \geq$ 3. We have used these FHI trigger values for secondary poisoning to clarify the guidance to $MAC_{eco, water}$ derivation:
  - As a guideline, a factor of 100 will be applied to the lowest L(E)C50 for substances having an experimentally determined BCF < 100 $L.kg_{ww}^{-1}$ and an experimentally determined BMF $\leq$ 1 $kg_{ww}.kg_{ww}^{-1}$ if available, or a log K_{ow} < 3 if no experimental BCF or BMF is available, provided that at least the base set is complete.
  - An assessment factor of 1000 will be applied to the lowest L(E)C50 for substances with an experimentally determined BCF $\geq$ 100 $L.kg_{ww}^{-1}$ or an experimentally determined BMF > 1 $kg_{ww}.kg_{ww}^{-1}$ or a log $K_{ow} \geq$ 3 if no experimental BCF or BMF is available, provided that at least the base set is complete.
  - Only in exceptional cases will a factor of 10 be applied. Such a factor must be backed up by the fact that acute toxicity data for different species do not differ by more than a factor of two to three (see also footnote d to Table 26).
  - There might be cases when the mode of toxic action is well known. If, in such case, there is a substantial amount of data for the most sensitive taxa, it might be considered to apply a factor of 10 in the case of non-bioaccumulative substances and 100 for bioaccumulative substances. In such a case it must be reasoned that the most sensitive species is protected by a high probability.

Table 26. Assessment factors to derive a $MAC_{eco, water}$.

Toxicity data	Additional information	Assessment factor
Base set not complete	–	– [a]
At least one short-term L(E)C50 from each of three trophic levels of the base set (fish, *Daphnia* and algae)	Potential to bioaccumulate [b]	1000
At least one short-term L(E)C50 from each of three trophic levels of the base set (fish, *Daphnia* and algae)	Potential to bioaccumulate [b]; AND known non-specific mode of action and low interspecies variation OR known mode of toxic action and most sensitive species included in data set	100
At least one short-term L(E)C50 from each of three trophic levels of the base set (fish, *Daphnia* and algae)	No potential to bioaccumulate [c]	100
At least one short-term L(E)C50 from each of three trophic levels of the base set (fish, *Daphnia* and algae)	No potential to bioaccumulate [c]; AND Acute toxicity data for different species do not differ by more than a factor 2 to 3 [d] OR known mode of toxic action and most sensitive species included in data set	10 [e]

Notes to Table 26.

a) When the base set is not complete, a $MAC_{eco, water}$ can not be derived.
b) Potential to bioaccumulate is defined as the substance having an experimental BCF $\geq$ 100 $L.kg_{ww}^{-1}$ or an experimental BMF > 1 $kg_{ww}.kg_{ww}^{-1}$ or, if BCF and BMF are absent, a log $K_{ow} \geq$ 3.
c) No potential to bioaccumulate is defined as the substance having an experimental BCF < 100 $L.kg_{ww}^{-1}$ and an experimental BMF $\leq$ 1 $kg_{ww}.kg_{ww}^{-1}$ or, if BCF and BMF are absent, a log K_{ow} < 3.
d) This guidance has been added within the INS framework. To assess the span of the acute toxicity data, all reliable acute toxicity data collected are used, with a minimum of three LC50 or EC50 values, for species representing each

of the base set trophic levels (algae, *Daphnia*, fish). If the ratio of the highest and lowest L(E)C50 value is ≤ 3, an assessment factor of 10 should be applied, otherwise an assessment factor of 100 should be applied.

e) Lowest assessment factor to be applied.

4.1.2 Derivation of $MAC_{eco, water}$ based on species sensitivity distributions

The FHI guidance also presents a method to base the risk limits for short-term exposure on the SSD method. For this purpose acute toxicity data are used.

- The same criteria with regard to the number of data, the taxonomic groups and the combination of freshwater and marine data are to be applied as for the use of the SSD method with chronic toxicity data (see section 3.1.2).
- An assessment factor is applied to the 5th percentile (median estimate) of the species sensitivity distribution to extrapolate from short-term L(E)C50 level to short-term no-effect level. The default value of this assessment factor is 10.
- Either a higher or a lower assessment factor than the default value of 10 may be used if this is required. Deviating from the default value should be justified. Take the acute-to-chronic ratio of the substance and the points for determination of the assessment factor for the SSD with chronic toxicity data (see section 3.1.2.3) into consideration.

4.1.3 Derivation of $MAC_{eco, water}$ based on simulated ecosystem studies

The FHI guidance on the use of micro- or mesocosm studies for the derivation of $MAC_{eco, water}$ is not straightforward and rather incomplete on several points. First, a citation from the FHI guidance is given, after which guidance for $MAC_{eco, water}$ derivation is given in section 4.1.3.1. An alternative method put forward by FHI, which is not supported by INS, is also explained in section 4.1.3.2.

FHI citation, p. 35, point 4.

'It may be possible to use the EAC, respectively NOEAEC, derived in Higher-Tier studies as MAC-EQS in certain cases. However, a thorough evaluation of the study results and the expected exposure pattern of the active substance in draining water bodies of a catchment area is required prior to the adoption of a EAC/NOEAEC as MAC-QS. Time needed to recover from impacts (if any) versus the probability that concentrations that caused the observed effects will recur is the decisive criterion. Ideally, a MAC-QS based on a Higher-Tier simulated ecosystem study should be the highest initial concentration that caused neither long-term nor ecologically relevant short-term effects in that study.'

'It is suggested to consider slight transient effects on functional parameters such as pH or oxygen content not as relevant if no concomitant effects on the investigated species could be observed. Effects on community structure (i.e. the populations of investigated species) may be regarded as not ecologically relevant if complete recovery of affected species occurs within the time interval over that short-term toxicity tests for the affected taxa normally are conducted (e.g. 72 h for algae, 48 h for daphnia, etc.).'

End of citation

4.1.3.1 Preferred method for $MAC_{eco, water}$ derivation using micro- or mesocosm studies

Deriving the NOEC from available studies.

The key sentence is that 'Ideally, a MAC-QS based on a Higher-Tier simulated ecosystem study should be the highest initial concentration that caused neither long-term nor ecologically relevant short-term effects', which is repeated in section 4.3.6.3 of the FHI document (with the exceptions mentioned in the last section of the above citation from section 4.3.5.1. of the FHI document).

In principle, these concentrations come closest to the protection level that the $MAC_{eco, water}$ should represent (neither long-term nor ecologically relevant short-term effects). In terms of the classes

from the Guidance Document on Aquatic Ecotoxicology (European Commission, 2002) only class 1 and class 2 are considered appropriate for the derivation of $MAC_{eco, water}$, similar to the derivation of the $MPC_{eco, water}$ (see section 3.1.2.4). The difference in the data that are considered suitable for these ERLs lies in the exposure concentrations, which should be initial concentrations for the $MAC_{eco, water}$ and time-weighted average concentrations for the $MPC_{eco, water}$. For the derivation of the $MAC_{eco, water}$ from micro- or mesocosm studies refer to section 3.1.2.4.

4.1.3.2 Alternative method for $MAC_{eco, water}$ derivation using micro- or mesocosm studies

This section elaborates on the first part of the FHI citation on p.35, point 4. For reasons of clarity we repeat the lines that are dealt with in the current section.

FHI citation
'It may be possible to use the EAC, respectively NOEAEC, derived in Higher-Tier studies as MAC EQS in certain cases. However, a thorough evaluation of the study results and the expected exposure pattern of the active substance in draining water bodies of a catchment area is required prior to the adoption of a EAC/NOEAEC as MAC-QS. Time needed to recover from impacts (if any) versus the probability that concentrations that caused the observed effects will recur is the decisive criterion'.
End of citation

Generally, the EAC or the NOEAEC can not be considered as: the highest initial concentration that caused neither long-term nor ecologically relevant short-term effects, which follows from the definitions of these parameters.

The NOEAEC is defined as 'the concentration at or below which no long-lasting adverse effects were observed in a particular higher-tier study (e.g. mesocosm). No long-lasting effects are defined as those effects on individuals that have no or only transient effects on populations and communities and are considered of minor ecological relevance (e.g., effects that are not shown to have long-term effects on population growth, taking into account the life-history characteristics of the organisms concerned). Different recovery rates may therefore be acceptable for different types of organisms' (European Commission, 2002). The NOEAEC is a concentration at which effects are not excluded in principle and therefore FHI deems it to be not or less useful as $MAC_{eco, water}$.

The EAC is defined as the 'concentration at or below which no ecologically adverse effects would be expected' (European Commission, 2002). Characteristics of the EAC are that it may have been derived by the use of an assessment factor, may be based on expert judgement and on more than one study. Since the definition of the EAC allows for ecologically adverse effects at the level of the EAC (i.e. not only below the level of the EAC), this is not compatible with the goal of the environmental quality standard ($MAC_{eco, water}$), which aims to exclude these effects. Therefore, FHI also deems the EAC to be less useful for setting of the $MAC_{eco, water}$.

Only in the case that an EAC or an NOEAEC will be used for $MAC_{eco, water}$ setting, FHI prompts incorporating information on exposure of the investigated substance. No further detail is given on this topic, which, in our opinion, is highly insufficient to serve as guidance. First, the notion that the exposure pattern of a substance is of importance for the setting of a $MAC_{eco, water}$ applies to all substances, not only those for which micro- or mesocosm studies are available. Second, no guidance is provided on how information on concentration peaks should be used to determine the height of the $MAC_{eco, water}$. Sampling frequency is highly important for the usefulness of data in this respect, but this is not dealt with. And third, $MAC_{eco, water}$ derivation becomes increasingly impracticable, since it demands complete accessibility to this type of data in representative water

bodies over extended periods (months, years). Fourth, an ERL should be a generic standard, which should be protective in all cases (within its definition). It should not be made dependent on emission or exposure patterns. In summary, we strongly advise not to incorporate, in INS framework, the exposure pattern of a substance in the $MAC_{eco, water}$ derivation.

4.1.4 Lower and upper limit of the $MAC_{eco, water}$ – additional INS guidance

4.1.4.1 Lower limit of the $MAC_{eco, water}$

The $MAC_{eco, water}$ may turn out to be lower than the $MPC_{eco, water}$. This can be caused by the use of different assessment factors in the derivation of these two ERLs. It is more likely to occur for those compounds that have a lowest acute toxicity test result (LC50 or EC50) which is close to the lowest chronic value (NOEC or EC10) in the toxicity data set.

$MAC_{eco, water}$ values below the MPC are not deemed realistic, since this would imply that one expects acute toxic effects at concentrations below the ERL that protects from chronic exposure. Therefore, in those cases where the $MAC_{eco, water}$ is lower than the $MPC_{eco, water}$, the $MAC_{eco, water}$ is set equal to the $MPC_{eco, water}$. This is in line with the recommendation in the report 'Towards the Derivation of Quality Standards for Priority Substances in the Context of the Water Framework Directive' (Lepper, 2002).

4.2 Derivation of NC

The following definition is given for the negligible concentration (NC):
'The target value (ed.: the EQS) is, in principle, set at the level of negligible concentration (NC) and is the guideline for the long-term environmental quality to be achieved. The NC has been set to a factor of 100 below the MPC, which defines a safety margin allowing for combination toxicity. The following points of departure have been used to derive target values:

- Protection of the ecological function: risks to ecosystems must be negligible
- Protection of functional properties of the environment: the use functions must be safeguarded'

With this definition and the accompanying definition of the MPC (see section 1.5), it is unclear whether ecotoxicological as well as human-toxicological endpoints should be taken into account for the derivation of the negligible concentration. Thus, in principle the NC is derived by dividing the final integrated MPC for the compartments water, groundwater, soil, sediment and air by a factor of 100. In the former INS guidance by Traas (2001), the NC only referred to the value for ecosystems, where it was stated that the NC represents a concentration at which only negligible effects on the ecosystem are expected.

For metals and other compounds that occur naturally in the environment, the NC can be calculated by means of the added risk approach, similar to the derivation of the MPC. The NC is defined as the background concentration (C_b) plus the Negligible Addition (NA) from the maximum permissible addition (MPA):

$$NC = C_b + NA \qquad (66)$$

$$NA = \frac{MPA}{100} \qquad (67)$$

4.3 Derivation of SRC_{eco}

For derivation of the SRC_{eco} both acute and chronic toxicity data should be tabulated. In general, the SRC_{eco} is the geometric mean of all available chronic toxicity data. When no or few chronic data are available, a comparison is made with the geometric mean of acute toxicity data. From the ecotoxicological evaluation of the first *tranche* of intervention values (Verbruggen *et al.*, 2001) up to now, the comparison between acute and chronic toxicity data was always made, unless the requirements for statistical extrapolation were fulfilled. However, at that time the guidance of the TGD had not yet been implemented with respect to this part of the derivation of the MPC. Statistical extrapolation was allowed if four or more taxonomic groups, regardless of which ones, were available. To bring the derivation of the SRC_{eco} more in line with the new guidance for the derivation of the MPC, the guidance for the comparison of acute and chronic toxicity data and the application of equilibrium partitioning was modified. The factors and conditions used for deriving SRC_{eco} are shown in Table 27 and Table 28.

- In principle, an acute-to-chronic ratio (ACR) of 10 is applied to the acute toxicity data to compare acute L(E)C50s with chronic NOECs (or EC10s). In the future, one may deviate from this factor of 10 if more information on the ACR for the specific compound or endpoint can be involved (Verbruggen *et al.*, 2001).
- For the aquatic compartment, comparison between chronic data and acute data is not performed when chronic data are available for *at least* three species, which should represent the three specified trophic levels from the base set of the TGD: algae, *Daphnia* and fish (see Table 27).
- For the sediment and terrestrial compartment, comparison between chronic data and acute data is not performed when chronic data are available for two species, each of which should represent a different trophic level, e.g. bacteria and earthworms, insects and macrophytes, molluscs and crustaceans. The same scheme is followed for both soil and sediment. In the derivation of MPCs for sediment, a comparison with EqP is not made at all when chronic toxicity data are available, even if there is only one NOEC or EC10. However, because the SRC_{eco} does not apply an assessment factor at all, the SRC_{eco} derived from a NOEC or EC10 for only one trophic level is also compared with a value derived by equilibrium partitioning.
- When the SRC_{eco} is to be reported with confidence limits, the computer program E_TX 2.0 (Van Vlaardingen *et al.*, 2004) is used to calculate the median HC_{50} and its 90% confidence interval. The HC_{50} is equal to the geometric mean of log-normally distributed toxicity data.
- The SRC_{eco} is always taken as the geometric mean of (either acute or chronic) toxicity data, irrespective of whether these data are log-normally distributed or not. If the data from which the SRC_{eco} is calculated do not fit a normal distribution, it suffices to note this briefly in the report section where the SRC_{eco} derivation is presented.
- Similar to the derivation of the MPC from the species sensitivity distribution, the data for single species and the data for microbial processes and enzymatic reactions are treated separately. For both types of data an SRC_{eco} is derived. The choice for the final SRC_{eco} is made on a case-by-case basis, but generally the lowest value will be selected.
- For metals the added risk approach should be followed (section 3.6). The SRC_{eco} is defined as the background concentration plus the serious risk addition (SRA_{eco}):

$$SRC_{eco} = C_b + SRA_{eco} \qquad (68)$$

Table 27. Assessment factors used to derive the SRC_{eco} for the aquatic compartment.

Available test results	Additional criteria	SRC_{eco} based on	Assessment factor
only L(E)C50s and no NOECs		geometric mean of L(E)C50s	10
1 NOEC[1] available	**none** of three specified taxa[2] is represented	geometric mean of L(E)C50s	10
1 NOEC[1] available	one of three specified taxa[2] is represented AND geometric mean of L(E)C50s / 10 < NOEC value	geometric mean of L(E)C50s	10
1 NOEC[1] available	one of three specified taxa[2] is represented AND geometric mean of L(E)C50s / 10 ≥ NOEC value	NOEC value	1
≥ 2 NOECs[1] available	**None** of three specified taxa[2] is represented	geometric mean of L(E)C50s	10
≥ 2 NOECs[1] available	one or two of three specified taxa[2] is represented AND geometric mean of L(E)C50s / 10 < geometric mean[3] of NOECs	geometric mean of L(E)C50s	10
≥ 2 NOECs[1] available	one or two of three specified taxa[2] is represented AND geometric mean of L(E)C50s / 10 ≥ geometric mean[3] of NOECs	geometric mean[3] of NOECs	1
≥ 3 NOECs[1] available	≥ 3 of three specified taxa[2] are represented	geometric mean[3] of NOECs	1

[1]This may also be an EC10 value.
[2]The 3 trophic levels for which NOEC data (and/or EC10 values) should be available are **algae, *Daphnia* and fish**.
[3]The geometric mean of all available NOECs (and/or EC10 values) is calculated; including the values that do not belong to the specified taxa.

Table 28. Assessment factors used to derive the SRC_{eco} for the soil and sediment compartment.

Available test results	Additional criteria	SRC_{eco} based on	Assessment factor
only L(E)C50 value(s) and no NOECs	comparison with EqP[1]	geometric mean of L(E)C50s	10
1 NOEC value[2]	comparison with EqP and acute toxicity data[3]	NOEC value	1
≥ 2 NOEC values[2, 4]	–	geometric mean of NOEC values	1

[1]If only acute data are available, the SRC_{eco} is also calculated on the basis of equilibrium partitioning. The lowest of both values is selected as SRC_{eco}.
[2]This may also be (an) EC10 value(s).
[3]If chronic toxicity data are available for only one trophic level, the SRC_{eco} is also calculated from the acute toxicity data, if available, and on basis of equilibrium partitioning. The lowest of these values is selected as SRC_{eco}.
[4]When chronic data are available, these data prevail and acute data are no longer used in SRC_{eco} derivation if these data NOECs are from different trophic levels.

5. Derivation of ERLs based on EU-RARs

For the compounds for which a finalised EU-RAR is available, ERL derivation should be carried out according to the procedure outlined in this section. Derivation of Dutch ERLs based on an EU-RAR was the subject of an earlier RIVM report (Janssen *et al.*, 2004). Parts of the procedure as described in Janssen *et al*. will be cited in this chapter.

5.1 MPC

5.1.1 MPC_{water}

- The $PNEC_{water}$ as reported in the EU-RAR is adapted as MPC_{water}. In general, the $PNEC_{water}$ is expressed as a dissolved value ($PNEC_{water, dissolved}$), which thus results in an $MPC_{water, dissolved}$. The $PNEC_{water}$ will be expressed as $PNEC_{water, total}$ only in exceptional cases (check the description of the critical study in the EU-RAR for those cases).
- According to the FHI guidance, the outcomes of aquatic toxicity studies should be regarded as total concentrations (see section 3.1.7.1, point 2). This means that the $PNEC_{water, dissolved}$ ($MPC_{water, dissolved}$) should be regarded as MPC_{water} without further recalculation; this value reflects a total concentration.
- If the substance interest has a log $K_{p, susp\text{-}water} \geq 3$, the MPC should also be expressed as a concentration in suspended matter ($MPC_{susp, water}$) using the guidance given in section 3.1.8.

5.1.2 MPC_{soil}

The $PNEC_{soil}$ as reported in the EU-RAR is taken over as MPC_{soil}. However, the MPC_{soil} should be recalculated to a value expressed in (dry weight) Dutch standard soil.

- Use equation 64 to recalculate MPC_{soil} from wet weight to dry weight, if necessary.
- Use procedures as described in section 3.7.4 for recalculation to Dutch standard soil.

In the cases where it is not possible to recalculate the MPC_{soil} to dry weight Dutch standard soil, this should be explicitly mentioned when reporting the ERL derivation. This MPC should be marked with a footnote in all tables where final MPC values are reported.

5.1.3 $MPC_{sediment}$

The $PNEC_{sediment}$ as reported in the EU-RAR is taken over as $MPC_{sediment}$. However, the $MPC_{sediment}$ should be recalculated to a value expressed in (dry weight) Dutch standard sediment.

- Use equation 62 to recalculate $MPC_{sediment}$ from wet weight to dry weight.
- Use procedures as described in section 3.7.4 for recalculation to Dutch standard sediment.

In the cases where it is not possible to recalculate the $MPC_{sediment}$ to dry weight Dutch standard sediment, this should be explicitly mentioned when reporting the ERL derivation. This MPC should be marked with a footnote in all tables where final MPC values are reported.

5.2 NC

The NC is derived from the MPC as described in section 4.1.

5.3 SRC_{eco}

The SRC_{eco} is derived using all reliable toxicity data collected in the EU-RAR with the methodology described in section 4.3.

6. Taxonomic classification of species in ERL derivation

6.1 Taxa

The purpose of Table 29 is to show the major taxonomic division in kingdoms and phyla for those organisms regularly encountered in ecotoxicological tests. Since taxonomy of species is a field of discipline which is in continuous development and various classification systems exist within biology, we do not aim for completeness here. We have followed the taxonomy as outlined in Lawrence (1996). Listed in the far right-hand column are the taxon names that are used to group species within the INS project framework. Two tables are presented on the following pages that show a further division of the presented phyla and the taxonomic groups discerned for use within the INS project. The taxonomic classification outlined in this section is in accordance with the TGD.

Table 29. Taxonomic position of test organisms I: kingdoms and phyla and classification within INS.

REGNUM	Common name	PHYLUM/DIVISION	Common name	INS-taxon
MONERA	Prokaryotes			
		GRACILICUTES		see Table 30
		MENDOSICUTES		see Table 30
PROTISTA	Protists			
		EUGLENOPHYTA	Euglenoids	Algae
		HETEROKONTOPHYTA		Algae
		CHLOROPHYTA	green algae	Algae
		MASTIGOPHORA	Flagellates	Protozoa
		SARCODINA (AMOEBAE)	Amoebas	Protozoa
		CILIOPHORA	Ciliates	Protozoa
PLANTAE	Plants			
		HEPATOPHYTA	Liverworts	
		ANTHOCEROPHYTA	Hornworts	
		BRYOPHYTA	Mosses	Bryophyta
		ANTOPHYTA	flowering plants	Macrophyta
MYCETAE	Fungi			
		ZYGOMYCOTA		Fungi
		ASCOMYCOTA		Fungi
		BASIDIOMYCOTA		Fungi
		DEUTEROMYCOTA		Fungi
ANIMALIA	Animals			
		PORIFERA	Sponges	Porifera
		CNIDARIA	corals, sea	Cnidaria
		CTENOPHORA		Ctenophora
		PLATYHELMINTES	Flatworms	Platyhelminthes
		GASTROTRICHA		Gastrotricha
		ROTIFERA	rotifers (wheel	Rotifera
		NEMATODA	nematodes,	Nematoda
		MOLLUSCA	Molluscs	Mollusca
		ANNELIDA	ringed worms	Annelida
		ARTHROPODA	Arthropods	see Table 30
		ECHINODERMATA	echinoderms	Echinodermata
		HEMICHORDATA		Hemichordata
		CHORDATA	vertebrates	see Table 30

Table 30 shows a more detailed taxonomic classification compared to Table 29 for those taxa that are further subdivided for INS purposes. Listed in the right column are the taxon names that are used to group species within the INS project framework.

Table 30. Taxonomic position of test organisms II: from kingdom to order and classification within INS.

REGNUM	**PHYLUM**	common name	**sub phylum**	**super class**	**class**	common name	**sub class**	**order**	common name	**INS-taxon name**
MONERA										
	EUBACTERIA									
					Scotophobia					Bacteria
					Oxyophotobacteria	cyanobacteria				Cyanobacteria
	ARCHAEBACTERIA									Archaebacteria
PROTISTA										
	DINOFLAGELLATA									Algae
	EUGLENOPHYTA	euglenoids								Algae
	HETEROKONTOPHYTA									
					Chrysophycae	golden algae				Algae
					Bacillariophycae	diatoms				Algae
	CHLOROPHYTA	green algae								Algae
	PROTOZOA									
			Sarcomastighophora							
				Mastigophora		flagellates				Protozoa
			Ciliophora			cilates				Protozoa
`PLANTAE			**Sarcodina**			amoebas				Protozoa
	HEPATOPHYTA	liverworts								
	ANTHOCEROPHYTA	hornworts								
	BRYOPHYTA	mosses								
	ANTOPHYTA	flowering plants								
	(MAGNOLIOPHYTA)									
					Dicotelydones					Macrophyta
					Monocotyledones					Macrophyta
MYCETAE		fungi								
	ZYGOMYCOTA									Fungi
	ASCOMYCOTA	e.g. yeasts, moulds								Fungi
	BASIDIOMYCOTA									Fungi
	DEUTEROMYCOTA	e.g. penicillum								Fungi
	MYCOPHYCOPHYTA	lichens								
ANIMALIA										
	PORIFERA	sponges								
	CNIDARIA									
	(COELENTERATA)									
					Anthozoa	corals and sea anemones				Cnidaria
					Hydrozoa	milliporine corals,				Cnidaria

REGNUM	PHYLUM	common name	sub phylum	super class	class	common name	sub class	order	common name	INS-taxon name
						hydroids, siphonophores				
					Scyphozoa	true jellyfishes				Cnidaria
	CTENOPHORA (COELERTERATA)									
					Tentacula					Ctenophora
					Nuda					Ctenophora
	PLATYHELMINTHES	flatworms								
					Turbellaria					Platyhelminthes
	GASTROTRICHA									Gastrostricha
	ROTIFERA	rotifers (wheel animals)								Rotifera
	NEMATODA	nematodes, roundworms								Nematoda
	MOLLUSCA	molluscs								
					Pelecypoda (Bivalvia)	Clams etc.				Mollusca
					Gastropoda					Mollusca
							Pulmonata		whelks, land and water snails, slugs etc.	Mollusca
					Scaphopoda	tusk shells				Mollusca
					Cephalopoda					Mollusca
	ANNELIDA	ringed worms								
					Oligochaeta	e.g. earthworms				Annelida
					Polychaeta	e.g. ragworms, lugworms				Annelida
					Hirudinae	leeches				Annelida
	ARTHROPODA	arthropods								
			Chelicerata		Arachnida					
								Araneida	spiders	Arachnida
								Acarina	ticks and mites	Arachnida
					Pycnogonida	sea spiders				Pycnogonida
			Crustacea							
					Branchiopoda	water fleas, etc.				Crustacea
					Ostracoda	ostracods				Crustacea
					Copepoda	copepods				Crustacea
					Mystacocarida					Crustacea
					Branchiura	fish lice				Crustacea
					Cirripedia	barnacles				Crustacea
					Malocostraca	crabs, lobsters, shrimps, woodlice				Crustacea
			Atelocerata							
					Diplopoda	millipedes				Myriapoda

REGNUM	PHYLUM	common name	sub phylum	super class	class	common name	sub class	order	common name	INS-taxon name
					Chilopoda	centipedes				Myriapoda
					Insecta	insects				
							Apterygota			
								Collembola	springtails	Insecta
							Pterygota			
								Odonata	dragonflies	Insecta
								Ephemeroptera	mayflies	Insecta
								Plecoptera	stoneflies	Insecta
								Trichoptera	caddis-flies	Insecta
								Coleoptera	beetles	Insecta
								Diptera	house flies, mosquitos, etc.	Insecta
								Hymenoptera	ants, wasps, bees	Insecta
	ECHINODERMATA	echinoderms								
			Pelmatozoa		Crinoidea	sea lillies, feather stars				Echinodermata
			Eleutherozoa		Stelleroidea	star fish, brittle stars				Echinodermata
					Echinoidea	sea urchins				Echinodermata
					Holothuroidea	sea cucumbers				Echinodermata
	HEMICHORDATA									
	CHORDATA									
			Urochordata (=Tunicata)							
			Cephalochordata			lancelets				
			Agnatha			jawless vertebrates				
			Gnatostomata			jawed vertebrates				
				Pisces		fishes				Pisces
					Chondrichthyes	sharks and rays				Pisces
					Osteichthyes	bony fishes				Pisces
				Tetrapoda						
					Amphibia	frogs, toads, salamanders, newts				Amphibia
					Reptilia					Reptilia
					Aves					Aves
					Mammalia					Mammalia

Some fish families that accommodate regularly tested species are: Salmonidae (including all *Salmo* and *Oncorhynchus* sp.), Cyprinidae (including *Carassius* sp., *Leuciscus* sp., *Brachydanio* sp., *Danio* sp., *Barbus* sp., *Rasbora* sp., *Phoxinus* sp.), Ictaluridae (*Ictalurus* sp.), Poeciliidae (e.g. *Poecilia* sp.) and Gasterosteidae (e.g. *Gasterosteus* sp.).

6.2 Trophic levels

6.2.1 Aquatic ecosystem

Appendix IV of the TGD (part II) may be consulted when the position of a taxonomic group in a trophic level of the aquatic ecosystem is needed. Three trophic levels are discerned: primary producers, primary consumers and secondary consumers. Appendix IV of the TGD is worked out for aquatic organisms only.

6.2.2 Terrestrial ecosystem

The trophic levels used in the TGD for the terrestrial ecosystem are primary producers, decomposers and consumers. Since little additional information is given on how to classify terrestrial organisms in these trophic levels, a more detailed classification in the following sections.

Primary producers
According to the TGD, the primary producers are plants (Macrophyta), producing food for heterotrophic organisms. We have extended this trophic level with Algae and Cyanobacteria, since there are many terrestrial, photoautotrophic species in both taxa that are also primary producers.

Decomposers
Decomposers contribute to the breakdown of organic matter (detritus, humus, litter) rather than predating on other organisms. The TGD mentions only Bacteria as ‘taxon’ in this trophic level. We have divided the level of decomposers in two separate classes: micro-organisms and higher organisms. The micro-organism decomposers operate at the molecular level: organic molecules are broken down into smaller fragments and/or eventually into inorganic nutrients. The higher organism decomposers fragment organic matter (litter, humus) or plants into smaller pieces.

Bacteria belong to the micro-organism decomposers. We have added the Fungi to this trophic level. Additionally, we discern the groups ‘Enzymatic reactions’ and ‘Microbial processes’ within the micro-organism decomposers. Ecotoxicological information for both groups is regularly encountered.
A few taxa are placed in the group of higher organism decomposers. The feeding strategy of these organisms can be characterised by breaking down organic material into smaller fragments. The food of these organisms is organic matter in various forms, or plant material, rather than other organisms (predation). The distinction between decomposers (higher organism) and consumers (next section) can not be made fully, since by consuming organic matter, the decomposers also eat bacteria and fungi and possibly other smaller organisms.

Consumers
The organisms at this level should be those that predominantly predate on other organisms. Species in this class will, to some extent, also digest organic matter.

Note that the classification given below is indicative. Especially the distinction between the decomposing higher organisms and the consumers may not be very sharp for some species. A species may be placed in a different category than indicated in the scheme when information on its feeding behaviour is available.

The indicative list of taxa below is divided over trophic levels for terrestrial organisms. Species listed are examples for which ecotoxicological data have been encountered.

Primary producers
- Algae (e.g. *Achnanthes* sp., *Ankistrodesmus* sp., *Chlamydomonas* sp., *Chlorella* sp., *Chlorococcum* sp., *Navicula* sp., *Nitzschia* sp., *Scenedesmus* sp., *Synedra* sp., *Ulothrix* sp.)
- Cyanobacteria (e.g. *Anabaena* sp., *Microcoleus* sp., *Nostoc* sp., *Oscillatoria* sp.)
- Macrophyta (all photosynthesising plant species)

Decomposers – micro-organisms
- Bacteria
- Enzymatic reactions[30] (e.g. amylase, dehydrogenase, glucosidase, invertase, phosphatase, sulphatase, urease)
- Microbial processes (e.g. denitrification, 'substrate'- mineralisation, nitrification, respiration, sulphur oxidation)
- Fungi
- Protozoa – saprobic feeders[31]

Decomposers – higher organisms
- Annelida (*Allolobophora* sp., *Aporrecrodea* sp., *Dendrobaena* sp., *Eisenia* sp., *Enchytraeus* sp[32]., *Lumbricus* sp.)
- Crustacea[33] (e.g. *Porcellio* sp., *Oniscus* sp.)
- Mollusca[34] (e.g. *Arianta* sp., *Arion* sp., *Helix* sp.)

Consumers
- Araneae (e.g. *Lycosa* sp., *Oedothorax* sp., *Paradosa* sp.)
- Acari (e.g. *Phytoseiulus* sp., *Platynothrus* sp., *Typhlodromus* sp.)
- Insecta (e.g. *Folsomia* sp., *Gryllus* sp., *Onychiurus* sp., *Orchesella* sp., *Poecilus* sp., *Tomocerus* sp.)
- Nematoda (e.g. *Aphelenchus* sp., *Caenorhabditis* sp., *Panagrellus* sp.)
- Protozoa – phagotrophic feeders[17]

[30] Soil enzymatic reactions are important in the ecological functioning of the soil. If toxicity data for these processes are available, they are taken into consideration in ERL derivation for the soil compartment.
[31] Although the dominant mode of protozoan nutrition in soil is considered to be phagotrophy (Lindal, 1990), sapbrobic feeding might be the most important route for some species. Check the feeding strategy for a given test organism in order to classify.
[32] Other species of enchytraeids may be encountered. Although several Enchytraeid species consume high amounts of fungal mycelium, they primarily decompose organic (plant) material (Lindal, 1990).
[33] Most terrestrial crustaceans are isopods (order Isopoda, suborder Oniscoideia). Although omnivores, the majority of their food consists of dead material (Lindal, 1990).
[34] Most terrestrial molluscs (Gastropoda) are generalist herbivores and many consume fungi (Lindal, 1990). They are placed in the comminutors by Römbke *et al*. (2003).

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Abbreviations, variables and default values

AA-QS	annual average quality standard
ACD	advanced chemistry development
ACR	acute to chronic ratio
ADI	acceptable daily intake
AF	assessment factor
ag	analytical grade
a.i.	active ingredient
am	artificial medium
ATSDR	agency for toxic substances and disease registry
AVS	acid volatile sulphide
BCF	bioconcentration factor
BLM	biotic ligand model
BMF	biomagnification factor
bw	body weight
CAS	chemical abstract service
CD	commission directive
CEPA	Canadian environmental protection act
CF	continuous flow system
c.i.	confidence interval
CICAD	concise international chemical assessment document
ClogP	log octanol/water partitioning coefficient, calculated by software program BioLoom
CMR	carcinogenic, mutagenic, reprotoxic
CTB	college toelating bestrijdingsmiddelen – Dutch board for the authorisation of pesticides
d	days
dfi	daily food intake
DG	directorate general
dtw	dechlorinated tap water
dw	de-ionised water, dechlorinated water or distilled water dry weight
DW	drinking water
DWQG	drinking-water quality guidelines
DWS	drinking-water standard
EAC	environmentally acceptable concentration
EC	European commission; effect concentration
ECB	European chemicals bureau
ECx	effect concentration at which an effect of x% is observed, generally EC10 and EC50 are calculated
EEC	European economic community (replaced by EU)
EHC	environmental health criteria
EINECS	European inventory of existing commercial chemical substances
ELS	early life stage
EPA	environmental protection agency
EPI	estimation programs interface
EPICS	equilibrium in partitioning in closed systems
EqP	equilibrium partitioning

EQS	environmental quality standard
ERL	environmental risk limit
ESIS	European chemical substances information system
EU	European union
EU-RAR	European union-risk assessment report
EUSES	European union system for the evaluation of substances
F	flow through system
FAO	food and agriculture organisation
FETAX	frog embryo teratogenesis assay
FHI	Fraunhofer Institute
FID	flame ionisation detection
GC	gas chromatography
GLP	good laboratory practice
h	hours
HC_x	hazardous concentration at which x percent of species is potentially affected
HPLC	high pressure liquid chromatography
HSDB	hazardous substances databank
HSG	health and safety guides
IARC	international agency for research on cancer
ICSC	international chemical safety cards
IF	intermittent flow system
INS	International and National Environmental Quality Standards for Substances in the Netherlands (In Dutch: (Inter)nationale Normen Stoffen)
IPCS	international programme on chemical safety
IRIS	integrated risk information system
ISO	international organisation for standardisation
IUCLID	international uniform chemical information database
IUPAC	international union of pure and applied chemistry
JECFA	joint expert committee on food additives
JMPR	joint meeting on pesticide residues
LCx	effect concentration at which x% lethality is observed, generally LC50 and LC10 are calculated
LD50	dose that is lethal to 50% of the tested animals
lg	laboratory grade
LSC	liquid scintillation counting
LOEC	lowest observed effect concentration
MAC	maximum acceptable concentration
MATC	maximum acceptable toxicant concentration
MCI	molecular connectivity indices
MlogP	log octanol/water partitioning coefficient, measured value selected by software program BioLoom
min	minutes
mo	months
MPA	maximum permissible addition
MPC	maximum permissible concentration
MRL	minimum risk level
mRNA	messenger ribonucleic acid
MS	mass spectrometry, Microsoft
NA	negligible addition
NC	negligible concentration

NIEHS	national institute of environmental health sciences
NIH	national institutes of health
NOEAEC	no observed ecologically adverse effect concentration
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NOEL	no observed effect level
NTP	national toxicology program (United States)
nw	natural water, such as lake water, river water, sea water, well water
oc	organic carbon
OECD	organisation for economic co-operation and development
OEHHA	office of environmental health hazard assessment
om	organic matter
OPPTS	office of prevention, pesticides and toxic substances
P5-COV	5^{th} percentile cut-off value
pa	pro analyse
PAH	polycyclic aromatic hydrocarbon
PCB	polychlorinated biphenyl
PEC	predicted environmental concentration
PNEC	predicted no effect concentration
PPP	plant protection product
ppt	parts per thousand or parts per trillion
psu	practical salinity unit
QS	quality standard
QSAR	quantitative structure activity relationship
R	renewal system
RA	risk assessment
RAR	risk assessment report
RfD	reference dose
rg	reagent grade
rtw	reconstituted tap water: tap water with additional salts
rw	reconstituted water: (natural) water with additional salts
RIVM	national institute for public health and the environment
S	static
Sc	static, closed system
SEC	expertise centre for substances
SEM	simultaneously extracted metals
SIDS	screening information data set
SMILES	simplified molecular input line entry system
sp.	species
SPARC	SPARC performs automatic reasoning in chemistry
SPMD	semi permeable membrane device
SPME	solid phase micro extraction
SRA_{eco}	ecotoxicological serious risk addition
SRC_{eco}	ecotoxicological serious risk concentration
STP	sewage treatment plant
susp	suspended particulate matter
SSD	species sensitivity distribution
t/a	tonne per annum
TCA	tolerable concentration in air
TCB	(Dutch) technical committee on soil protection

TDI	tolerable daily intake
TERA	toxicology excellence for risk assessment
tg	technical grade
TGD	Technical Guidance Document
TL	threshold level
TLm	median tolerance limit; also encountered as: median threshold limit
tw	tap water
TWA	time weighted average
UBA	Umweltbundesamt
UNEP	united nations environment programme
US	United States
UV	ultraviolet
VROM	Ministry of Housing, Spatial Planning and the Environment
w	weeks
WAF	water accommodated fraction
WFD	water framework directive
WHO	world health organisation
ww	wet weight
y	years

Table 31. List of defaults and variables used throughout the report.

Symbol	Description of variable	Unit	Value
10^{-6}	conversion factor from mg to kg	$kg.mg^{-1}$	
0.1	safety factor to account for uptake of maximally 10% of TL_{hh} (human toxicological threshold level)	–	
0.115	daily human consumption of fishery products	$kg.d^{-1}$	
5% SSD	5th percentile of the species sensitivity distribution	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
50% c.i.	median estimate, or: the value which has 50% probability of being exceeded	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
100	assessment factor to derive TL_{hh} from $NOEL_{min}$	–	
ADI	acceptable daily intake	$mg.kg_{bw}^{-1}.d^{-1}$	
1000	conversion factor from m^3 to litre	$L.m^{-3}$	
AF	assessment factor	–	1-5
AF_{oral}	assessment factor applied in extrapolation of *MPC*	–	
ALPHA	sink term of differential equation	d^{-1}	
$AREA_{plant}$	leaf surface area	m^2	5
b	correction exponent for differences between plant lipids and octanol	-	0.95
BAF_{meat}	bioaccumulation factor for meat	$d.kg_{meat}^{-1}$	
BAF_{milk}	bioaccumulation factor for milk	$d.kg_{milk}^{-1}$	
$BCF_{earthworm}$	bioconcentration factor for earthworm on wet weight basis	$L.kg_{ww}^{-1}$	
BCF_{fish}	bioconcentration factor for fish on wet weight basis	$L.kg_{ww}^{-1}$	
BCF_{mussel}	bioconcentration factor for mussels on wet weight basis	$L.kg_{ww}^{-1}$	
$BETA_{agric}$	source term of differential equation for crops	$kg_c.m^{-3}.d^{-1}$	
$BETA_{grass}$	source term of differential equation for grass	$kg_c.m^{-3}.d^{-1}$	
BMF_1	biomagnification from (small) fish to predators		
BMF_2	biomagnification factor from predators to top predators		
$BSAF_{earthworm}$	biota (earthworm) to soil accumulation factor	$kg_{dw}.kg_{ww}^{-1}$	
BW	human body weight	kg_{bw}	70
C_{air}	concentration in air	$kg.m^{-3}$	
$C_{agric,porew\ leaf}$	concentration in pore water of agricultural soil, calculated from C_{leaf}	$kg.m^{-3}$	
$C_{agric,porew\ root}$	concentration in pore water of agricultural soil, calculated from C_{root}	$kg.m^{-3}$	
C_b	background concentration	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
$C_{b,\ dissolved}$	background concentration expressed as dissolved fraction	$mg.L^{-1}$	
$C_{b,\ susp}$	background concentration expressed in particulate matter	$mg.kg^{-1}$	
$C_{b,\ total}$	background concentration expressed as total concentration	$mg.L^{-1}$	
%clay	clay content	% (w/w)	
C_{grass}	concentration in grass (wet weight)	$kg.kg_{ww}^{-1}$	
$C_{grassland}$	concentration in the soil beneath grassland	$kg.kg_{ww}^{-1}$	
$C_{grassland,\ porew}$	concentration in pore water of grassland	$kg.m^{-3}$	
C_{leaf}	concentration in leaves of plant	$kg.kg_{ww}^{-1}$	
C_{meat}	concentration in meat	$kg.kg_{ww}^{-1}$	
C_{milk}	concentration in dairy products	$kg.kg_{ww}^{-1}$	
C_{root}	concentration in root tissue of plant	$kg.kg_{ww}^{-1}$	
C_{soil}	concentration in soil corresponding with $C_{agric,\ porew\ leaf}$ via EqP	$kg.kg_{ww}^{-1}$	
$CONV_{bird}$	conversion factor from NOAEL to NOEC	$kg_{bw}.d.kg_{food}^{-1}$	
$CONV_{grass}$	conversion factor grass from dry weight to wet weight	$kg_{ww}.kg_{dw}^{-1}$	
$CONV_{mammal}$	conversion factor from NOAEL to NOEC	$kg_{bw}.d.kg_{food}^{-1}$	
$CONV_{soil}$	*conversion factor for soil concentration wet-dry weight soil*	$kg_{ww}.kg_{dw}^{-1}$	
$C\text{porew}_{comp}$	total concentration in pore water of compartment comp	$mg.m^{-3}$	
C_{susp}	concentration of suspended matter in surface water	$mg.L^{-1}$	

Symbol	Description of variable	Unit	Value
$C_{susp,\ Dutch\ standard}$	concentration of suspended particulate matter in fresh water based on Dutch standard particulate matter characteristics	$mg.L^{-1}$	30
$C_{susp\ marine,\ FHI}$	concentration of suspended particulate matter in marine water sample used in FHI guidance	$mg.L^{-1}$	3
$C\text{total}_{comp}$	total concentration in compartment comp	$mg.m^{-3}$	
DWstandard (CD 98/83/EC)	drinking-water standard according to CD 98/83/EC	$mg.L^{-1}$	
EC_x	effect concentration exerting x% effect	$mg.L^{-1}$	
$F\text{air}_{comp}$	fraction air in compartment comp (only relevant for soil)	$m^3.m^{-3}$	
$F\text{air}_{plant}$	volume fraction of air in plant tissue	$m^3.m^{-3}$	0.3
$F\text{air}_{soil}$	fraction air in soil	$m^3.m^{-3}$	0.2
$F\text{air}_{susp}$	fraction air in suspended matter	$m^3.m^{-3}$	0
$F\text{ass}_{aer}$	fraction of substance adsorbed to aerosol	-	
F_{gut}	fraction of gut loading in earthworm	$kg_{dw}.kg_{ww}^{-1}$	0.1
$F\text{lipid}_{plant}$	volume fraction of lipids in plant tissue	$m^3.m^{-3}$	0.01
$F_{not\ removable\ by\ simple\ treatment}$	fraction not removable by simple treatment	–	
$F\text{oc}_{comp}$	weight fraction of organic carbon in compartment comp	$kg.kg^{-1}$	
$F\text{oc}_{Dutch\ standard\ sediment}$	fraction organic carbon in Dutch standard sediment	$kg.kg^{-1}$	0.0588
$F\text{oc}_{Dutch\ standard\ soil}$	fraction organic carbon in Dutch standard soil	$kg.kg^{-1}$	0.0588
$F\text{oc}_{Dutch\ standard\ susp}$	fraction organic carbon in Dutch standard soil	$kg.kg^{-1}$	0.1176
$F\text{oc}_{soil}$	weight fraction of organic carbon in soil	$kg.kg^{-1}$	
$F\text{oc}_{soil,\ TGD}$	weight fraction of organic carbon in soil as defined in the TGD	$kg.kg^{-1}$	0.02
$F\text{oc}_{susp,\ TGD}$	weight fraction of organic carbon in suspended matter as defined in the TGD	$kg.kg^{-1}$	0.1
$F\text{om}_{experimental\ sediment}$	fraction organic matter in experimental sediment	$kg.kg^{-1}$	
$F\text{om}_{experimental\ soil}$	fraction organic matter in experimental soil	$kg.kg^{-1}$	
$F\text{om}_{Dutch\ standard\ sediment}$	fraction organic matter in Dutch standard sediment	$kg.kg^{-1}$	0.1
$F\text{om}_{Dutch\ standard\ soil}$	fraction organic matter in Dutch standard soil	$kg.kg^{-1}$	0.1
$F\text{om}_{Dutch\ standard\ susp}$	fraction organic matter in Dutch standard suspended matter	$kg.kg^{-1}$	0.2
$F\text{solid}_{comp}$	fraction solids in compartment comp	–	
$F\text{solid}_{soil}$	fraction solids in soil	$m^3.m^{-3}$	0.6
$F\text{solid}_{susp}$	fraction solids in suspended matter	$m^3.m^{-3}$	0.1
$F_{TDI,\ root}$	allowable fraction of TDI to be filled by root crop consumption	–	0.1
$F_{TDI,\ leaf}$	allowable fraction of TDI to be filled by leaf crop consumption	–	0.1
$F_{TDI,\ meat}$	allowable fraction of TDI to be filled by meat consumption	–	0.1
$F_{TDImilk}$	allowable fraction of TDI to be filled by dairy product consumption	–	0.1
$F\text{water}_{comp}$	fraction water in compartment comp	$m^3.m^{-3}$	
$F\text{water}_{plant}$	volume fraction of water in plant tissue	$m^3.m^{-3}$	0.65
$F\text{water}_{soil}$	fraction water in compartment soil	$m^3.m^{-3}$	0.2
$F\text{water}_{susp}$	fraction water in compartment susp	$m^3.m^{-3}$	0.9
g_{plant}	leaf conductance (0.001 $m.s^{-1}$)	$m.d^{-1}$	86.4
H	Henry's law constant	$Pa.m^3.mol^{-1}$	
$HC_{5,\ median}$	median estimate of the 5th percentile of the SSD	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
$IC\text{dwt}_{grass}$	daily intake for cattle of grass (dry weight)	$kg_{ww}.d^{-1}$	16.9
$IC\text{dwt}_{soil}$	daily intake of soil (dry weight)	$kg_{ww}.d^{-1}$	0.41
IC_{grass}	daily intake of grass (wet weight)	$kg_{ww}.d^{-1}$	
IC_{soil}	daily intake of soil (wet weight)	$kg_{ww}.d^{-1}$	
IH_{leaf}	daily intake of leaf crops (incl. fruit and cereals)	$kg_{ww}.d^{-1}$	1.2
IH_{meat}	daily intake of meat	$kg_{ww}.d^{-1}$	0.301
IH_{milk}	daily intake of dairy products	$kg_{ww}.d^{-1}$	0.561
IH_{root}	daily intake of root crops	$kg_{ww}.d^{-1}$	0.384
$K_{air\text{-}water}$	air-water partition coefficient	$m^3.m^{-3}$	
$K_{comp\text{-}water}$	partition coefficient between compartment and water	$m^3.m^{-3}$	

Symbol	Description of variable	Unit	Value
$kelim_{plant}$	rate constant for total elimination in plants	d^{-1}	
$kgrowth_{plant}$	pseudo first order rate constant for dilution by growth	d^{-1}	0.035
$kmetab_{plant}$	pseudo first order rate constant for metabolism in plants	d^{-1}	0
$kphoto_{plant}$	pseudo first order rate constant for photolysis in plants	d^{-1}	0
$K_{leaf\text{-}air}$	partition coefficient between leaves and air	$m^3.m^{-3}$	
$K_{plant\text{-}water}$	partition coefficient between plant tissue and water	$m^3.m^{-3}$	
Kp_{soil}	solids-water partition coefficient in soil	$m^3.kg^{-1}$	
$K_{soil\text{-}water}$	total soil-water partition coefficient	$m^3.m^{-3}$	
K_{ow}	*n*-octanol water partition coefficient	–	
K_{oc}	partition coefficient between organic carbon and water	$L.kg^{-1}$	
K_p	partition coefficient	$L.kg^{-1}$	
Kp_{comp}	partition coefficient solids-water in compartment comp	$L.kg^{-1}$	
Kp_{sed}	partition coefficient solid-water in sediment	$L.kg^{-1}$	
Kp_{soil}	partition coefficient solid-water in soil	$L.kg^{-1}$	
$K_{p,\ susp\text{-}water}$	partition coefficient between suspended matter and water	$L.kg^{-1}$	
Kp_{susp}	partition coefficient solid-water in suspended matter	$L.kg^{-1}$	
$K_{sed\text{-}water}$	sediment-water partition coefficient	$mg.m^{-3}$	
$K_{soil\text{-}water}$	soil-water partition coefficient	$mg.m^{-3}$	
$K_{susp\text{-}water}$	suspended matter-water partition coefficient	$mg.m^{-3}$	
MPA	maximum permissible addition (general term)	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
$MPA_{water,\ dissolved}$	maximum permissible addition in water, expressed as the dissolved part of the substance concentration in the water	$mg.L^{-1}$	
$MPA_{water,\ susp}$	maximum permissible addition in water, expressed as the substance concentration in suspended particulate matter	$mg.kg^{-1}$	
$MPA_{water,\ total}$	maximum permissible addition in water, expressed as the substance concentration in the total (unfiltered) water sample	$mg.L^{-1}$	
MPC	maximum permissible concentration (general term)	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
$MPC_{Dutch\ standard\ sediment,\ EqP,\ dw}$	maximum permissible concentration in sediment based on equilibrium partitioning, expressed in dry weight Dutch standard sediment	$mg.kg_{dw}^{-1}$	
$MPC_{Dutch\ standard\ soil,\ EqP,\ dw}$	maximum permissible concentration in soil based on equilibrium partitioning, expressed in dry weight Dutch standard soil	$mg.kg_{dw}^{-1}$	
$MPC_{dw,\ water,\ provisional}$	provisional value for the maximum permissible concentration for freshwater; based on drinking water	$mg.L^{-1}$	
$MPC_{eco,\ gw}$	maximum permissible concentration in groundwater based on ecotoxicity	$mg.L^{-1}$	
$MPC_{eco,\ marine}$	maximum permissible concentration in marine water based on ecotoxicity	$mg.L^{-1}$	
$MPC_{eco,\ water}$	maximum permissible concentration in freshwater based on ecotoxicity	$mg.L^{-1}$	
$MPC_{hh\ food}$	maximum permissible concentration for humans based on fish consumption	$mg.kg_{food}^{-1}$	
$MPC_{hh\ food,\ water}$	maximum permissible concentration in freshwater based on human fish consumption	$mg.L^{-1}$	
MPC_{human}	maximum permissible concentration for humans	$mg.kg_{bw}^{-1}.d^{-1}$ or equivalent	
$MPC_{human,\ gw}$	maximum permissible concentration in groundwater based on drinking-water consumption	$mg.L^{-1}$	
$MPC_{human,soil\ leaf}$	maximum permissible concentration in soil based on leaf consumption	$mg.kg^{-1}$ or equivalent	
$MPC_{human,soil\ meat}$	maximum permissible concentration in soil based on meat consumption	$mg.kg^{-1}$ or equivalent	
$MPC_{human,soil\ milk}$	maximum permissible concentration in soil based on milk consumption	$mg.kg^{-1}$ or equivalent	

Symbol	Description of variable	Unit	Value
$MPC_{human,soil\ root}$	maximum permissible concentration in soil based on root consumption	$mg.kg^{-1}$ or equivalent	
MPC_{marine}	maximum permissible concentration in marine water; overall MPC for marine water	$mg.L^{-1}$	
$MPC_{marine\ sediment}$	maximum permissible concentration in marine sediment	$\mu g.kg_{dw}^{-1}$	
$MPC_{marine,\ total}$	maximum permissible concentration for marine water referring to the substance concentration in the total (unfiltered) water sample	$mg.L^{-1}$	
$MPC_{oral,\ bird}$	maximum permissible concentration for birds via oral route	$mg.kg_{food}^{-1}$	
$MPC_{oral,\ mammal}$	maximum permissible concentration for mammals via oral route	$mg.kg_{food}^{-1}$	
$MPC_{oral,\ min}$	lowest MPC_{oral} derived from toxicity studies	$mg.kg_{food}^{-1}$	
$MPC_{sediment,\ TGD,\ EqP,\ dw}$	maximum permissible concentration in sediment based equilibrium partitioning, expressed in dry weight sediment with standard TGD characteristics	$\mu g.kg_{dw}^{-1}$	
$MPC_{sediment,\ TGD,\ EqP,\ ww}$	maximum permissible concentration in sediment based equilibrium partitioning, expressed in wet weight sediment with standard TGD characteristics	$\mu g.kg_{ww}^{-1}$	
$MPC_{soil,\ TGD,\ EqP,\ dw}$	maximum permissible concentration in soil based equilibrium partitioning, expressed in dry weight soil with standard TGD characteristics	$\mu g.kg_{dw}^{-1}$	
$MPC_{soil,\ TGD,\ EqP,\ ww}$	maximum permissible concentration in soil based equilibrium partitioning, expressed in wet weight soil with standard TGD characteristics	$\mu g.kg_{ww}^{-1}$	
$MPC_{sp,\ marine}$	maximum permissible concentration in marine water based on secondary poisoning	$mg.L^{-1}$	
$MPC_{sp,\ soil}$	maximum permissible concentration in soil based on secondary poisoning	$mg.kg^{-1}$	
$MPC_{sp,\ soil,\ TGD}$	maximum permissible concentration in soil based on secondary poisoning using TGD soil characteristics	$mg.kg^{-1}$	
$MPC_{sp,\ water}$	maximum permissible concentration in freshwater based on secondary poisoning	$mg.L^{-1}$	
$MPC_{susp,\ water}$	maximum permissible concentration for freshwater referring to the substance concentration in suspended particulate matter	$mg.kg^{-1}$	
MPC_{water}	maximum permissible concentration for freshwater; overall MPC for freshwater	$mg.L^{-1}$	
$MPC_{water,\ dissolved}$	maximum permissible concentration for freshwater referring to the dissolved part of the substance concentration in the water	$mg.L^{-1}$	
$MPC_{water,\ dw}$	maximum permissible concentration for freshwater; based on drinking water	$mg.L^{-1}$	
$MPC_{water,\ total}$	maximum permissible concentration for freshwater referring to the substance concentration in the total (unfiltered) water sample	$mg.L^{-1}$	
M_w	molecular weight	$g.mol^{-1}$	
NA	negligible addition	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
NC	negligible concentration	$mg.L^{-1}$ or $mg.kg^{-1}$ or equivalent	
$NOAEL_{bird}$	no observed adverse effect level for birds	$mg.kg_{bw}^{-1}.d^{-1}$	
$NOAEL_{oral\ human}$	no observed adverse effect level for humans	$mg.kg_{bw}^{-1}.d^{-1}$	
$NOAEL_{mammal,\ oral\_chr}$	no observed adverse effect level for mammals	$mg.kg_{bw}^{-1}.d^{-1}$	
$NOEC_{bird}$	no observed effect concentration for birds	$mg.kg_{food}^{-1}$	
$NOEC_{community}$	no observed effect concentration at the community level in mesocosm or field study	$mg.L^{-1}$	
$NOEC_{mammal,\ food\_chr}$	no observed effect concentration for mammals	$mg.kg_{food}^{-1}$	

Symbol	Description of variable	Unit	Value
$NOEC_{population}$	no observed effect concentration at the population level in mesocosm or field study	$mg.L^{-1}$	
$NOEL_{min}$	lowest available no observed effect level	$mg.kg_{bw}^{-1}.d^{-1}$	
%oc	organic carbon content	% (w/w)	
%om	organic matter content	% (w/w)	
pK_a	-log of dissociation constant	–	
PNEC	predicted no effect concentration	$mg^{.L-1}$ or $^{mg.kg-1}$ or equivalent	
P_v	vapour pressure	Pa	
Q	substitution factor		
Q_{transp}	transpiration stream	$m^3.d^{-1}$	0.001
R	gas constant	$Pa.m^3.mol^{-1}.K^{-1}$	8.314
$RHO_{earthworm}$	density of wet weight earthworm	$kg_{ww}^{.L-1}$	1
RHO_{plant}	bulk density of plant tissue (wet weight)	$kg_{ww}.m^{-3}$	700
RHO_{soil}	bulk density of wet soil	$kg_{ww}.m^{-3}$	1700
*RHO*solid	density of the solid phase	$kg_{solid}.m_{solid}^{-3}$	2500
RHO_{susp}	bulk density of wet suspended particulate matter	$kg_{ww}.m^{-3}$	1150
S	salinity	‰ = ppt ≈ psu	
SRA_{eco}	serious risk addition for the ecosystem	$mg^{.L-1}$ or $^{mg.kg-1}$ or equivalent	
SRC_{eco}	serious risk concentration for the ecosystem	$mg^{.L-1}$ or $^{mg.kg-1}$ or equivalent	
S_w	water solubility	$mg^{.L-1}$	
TDI	tolerable daily intake	$mg.kg_{bw}^{-1}.d^{-1}$	
TEMP	environmental temperature	K	285
$TEST\ RESULT_{Dutch\ standard\ sediment}$	LC50, EC50, NOEC, EC10 from sediment toxicity study, expressed in Dutch standard sediment	$mg.kg_{dw}^{-1}$	
$TEST\ RESULT_{Dutch\ standard\ soil}$	LC50, EC50, NOEC, EC10 from terrestrial toxicity study, expressed in Dutch standard soil	$mg.kg_{dw}^{-1}$	
$TEST\ RESULT_{experimental\ sediment}$	LC50, EC50, NOEC, EC10 from sediment toxicity study, expressed in experimental sediment	$mg.kg_{dw}^{-1}$	
$TEST\ RESULT_{experimental\ soil}$	LC50, EC50, NOEC, EC10 from terrestrial toxicity study, expressed in experimental soil	$mg.kg_{dw}^{-1}$	
TL_{hh}	threshold level for human health (ADI, TDI, $NOAEL_{oral}$/AF, etc.)	$mg.kg_{bw}^{-1}.d^{-1}$	
TOX_{oral}	either $LC50_{bird}$, $NOEC_{bird}$ or $NOEC_{mammal,\ food\_chr}$	$mg.kg_{food}^{-1}$	
TSCF	transpiration-stream concentration factor	-	
$Uptake_{dw}$	uptake drinking water	$L.d^{-1}$	2
V_{leaf}	shoot volume	m^3	0.002

Appendix 1: A1 values from Council Directive 75/440/EC

	Parameters		A1 G	A1 I
1	pH		6 5 to 8 5	
2	Coloration (after simple filtration)	mg/l Pt scale	10	20 (O)
3	Total suspended solids	mg/l SS	25	
4	Temperature	C	22	25 (O)
5	Conductivity	µs/cm^{-1} at 20 C	1 000	
6	Odour	(dilution factor at 25 C)	3	
7*	Nitrates	mg/l NO_3	25	50 (O)
8 (1)	Fluorides	mg/l F	0 7 to 1	1 5
9	Total extractable organic chlorine	mg/l Cl		
10*	Dissolved iron	mg/l Fe	0 1	0 3
11*	Manganese	mg/l Mn	0 05	
12	Copper	mg/l Cu	0 02	0 05 (O)
13	Zinc	mg/l Zn	0 5	3
14	Boron	mg/l B	1	
15	Beryllium	mg/l Be		
16	Cobalt	mg/l Co		
17	Nickel	mg/l Ni		
18	Vanadium	mg/l V		
19	Arsenic	mg/l As	0 01	0 05
20	Cadmium	mg/l Cd	0 001	0 005
21	Total chromium	mg/l Cr		0 05
22	Lead	mg/l Pb		0 05
23	Selenium	mg/l Se		0 01
24	Mercury	mg/l Hg	0 0005	0 001
25	Barium	mg/l Ba		0 1
26	Cyanide	mg/l Cn		0 05
27	Sulphates	mg/l SO_4	150	250
28	Chlorides	mg/l Cl	200	

	Parameters		A1 G	A1 I
29	Surfactants (reacting with methyl blue)	mg/l (laurylsulphate)	0 2	
30* (2)	Phosphates	mg/l P_2O_5	0 4	
31	Phenols (phenol index) paranitraniline 4 aminoantipyrine	mg/l C_6H_5OH		0 001
32	Dissolved or emulsified hydrocarbons (after extraction by petroleum ether)	mg/l		0 05
33	Polycyclic aromatic hydrocarbons	mg/l		0 0002
34	Total pesticides (parathion, BHC, dieldrin)	mg/l		0 001
35*	Chemical oxygen demand (COD)	mg/l O_2		
36*	Dissolved oxygen saturation rate	% O_2	> 70	
37*	Biochemical oxygen demand (BOD_5) (at 20 C without nitrification)	mg/l O_2	< 3	
38	Nitrogen by Kjeldahl method (except NO_3)	mg/l N	1	
39	Ammonia	mg/l NH_4	0 05	
40	Substances extractable with chloroform	mg/l SEC	0 1	
41	Total organic carbon	mg/l C		
42	Residual organic carbon after flocculation and membrane filtration (5 µ) TOC	mg/l C		
43	Total coliforms 37 C	/100 ml	50	
44	Faecal coliforms	/100 ml	20	
45	Faecal streptococci	/100 ml	20	
46	Salmonella		Not present in 5 000 ml	

I = mandatory.
G = guide.
O = exceptional climatic or geographical conditions.
* = see Article 8 (d).

(1) The values given are upper limits set in relation to the mean annual temperature (high and low).
(2) This parameter has been included to satisfy the ecological requirements of certain types of environment.

Appendix 2: DWS values from Council Directive 98/83/EC

PART B

Chemical parameters

Parameter	Parametric value	Unit	Notes
Acrylamide	0,10	µg/l	Note 1
Antimony	5,0	µg/l	
Arsenic	10	µg/l	
Benzene	1,0	µg/l	
Benzo(a)pyrene	0,010	µg/l	
Boron	1,0	mg/l	
Bromate	10	µg/l	Note 2
Cadmium	5,0	µg/l	
Chromium	50	µg/l	
Copper	2,0	mg/l	Note 3
Cyanide	50	µg/l	
1,2-dichloroethane	3,0	µg/l	
Epichlorohydrin	0,10	µg/l	Note 1
Fluoride	1,5	mg/l	
Lead	10	µg/l	Notes 3 and 4
Mercury	1,0	µg/l	
Nickel	20	µg/l	Note 3
Nitrate	50	mg/l	Note 5
Nitrite	0,50	mg/l	Note 5
Pesticides	0,10	µg/l	Notes 6 and 7
Pesticides — Total	0,50	µg/l	Notes 6 and 8
Polycyclic aromatic hydrocarbons	0,10	µg/l	Sum of concentrations of specified compounds; Note 9
Selenium	10	µg/l	
Tetrachloroethene and Trichloroethene	10	µg/l	Sum of concentrations of specified parameters
Trihalomethanes — Total	100	µg/l	Sum of concentrations of specified compounds; Note 10
Vinyl chloride	0,50	µg/l	Note 1

Note 1: The parametric value refers to the residual monomer concentration in the water as calculated according to specifications of the maximum release from the corresponding polymer in contact with the water.

Note 2: Where possible, without compromising disinfection, Member States should strive for a lower value.

For the water referred to in Article 6(1)(a), (b) and (d), the value must be met, at the latest, 10 calendar years after the entry into force of the Directive. The parametric value for bromate from five years after the entry into force of this Directive until 10 years after its entry into force is 25 µg/l.

Note 3: The value applies to a sample of water intended for human consumption obtained by an adequate sampling method[35] at the tap and taken so as to be representative of a weekly average value ingested by consumers. Where appropriate the sampling and monitoring methods must be applied in a harmonised fashion to be drawn up in accordance with Article 7(4). Member States must take account of the occurrence of peak levels that may cause adverse effects on human health.

Note 4: For water referred to in Article 6(1)(a), (b) and (d), the value must be met, at the latest, 15 calendar years after the entry into force of this Directive. The parametric value for lead from five years after the entry into force of this Directive until 15 years after its entry into force is 25 µg/l. Member States must ensure that all appropriate measures are taken to reduce the concentration of lead in water intended for human consumption as much as possible during the period needed to achieve compliance with the parametric value. When implementing the measures to achieve compliance with that value Member States must progressively give priority where lead concentrations in water intended for human consumption are highest.

Note 5: Member States must ensure that the condition that nitrate]/50 + nitrite]/3 # 1, the square brackets signifying the concentrations in mg/l for nitrate (NO_3) and nitrite (NO_2), is complied with and that the value of 0,10 mg/l for nitrites is complied with ex water treatment works.

Note 6: 'Pesticides' means:
— organic insecticides,
— organic herbicides,
— organic fungicides,
— organic nematocides,
— organic acaricides,
— organic algicides,
— organic rodenticides
— organic slimicides,
— related products (*inter alia*, growth regulators)
and their relevant metabolites, degradation and reaction products.

Only those pesticides which are likely to be present in a given supply need be monitored.

Note 7: The parametric value applies to each individual pesticide. In the case of aldrin, dieldrin, heptachlor and heptachlor epoxide the parametric value is 0,030 µg/l.

Note 8 'Pesticides — Total' means the sum of all individual pesticides detected and quantified in the monitoring procedure.

Note 9: The specified compounds are:
— benzo(b)fluoranthene,
— benzo(k)fluoranthene,
— benzo(ghi)perylene,
— indeno(1,2,3-cd)pyrene.

Note 10: Where possible, without compromising disinfection, Member States should strive for a lower value.

The specified compounds are: chloroform, bromoform, dibromochloromethane, bromodichloromethane.

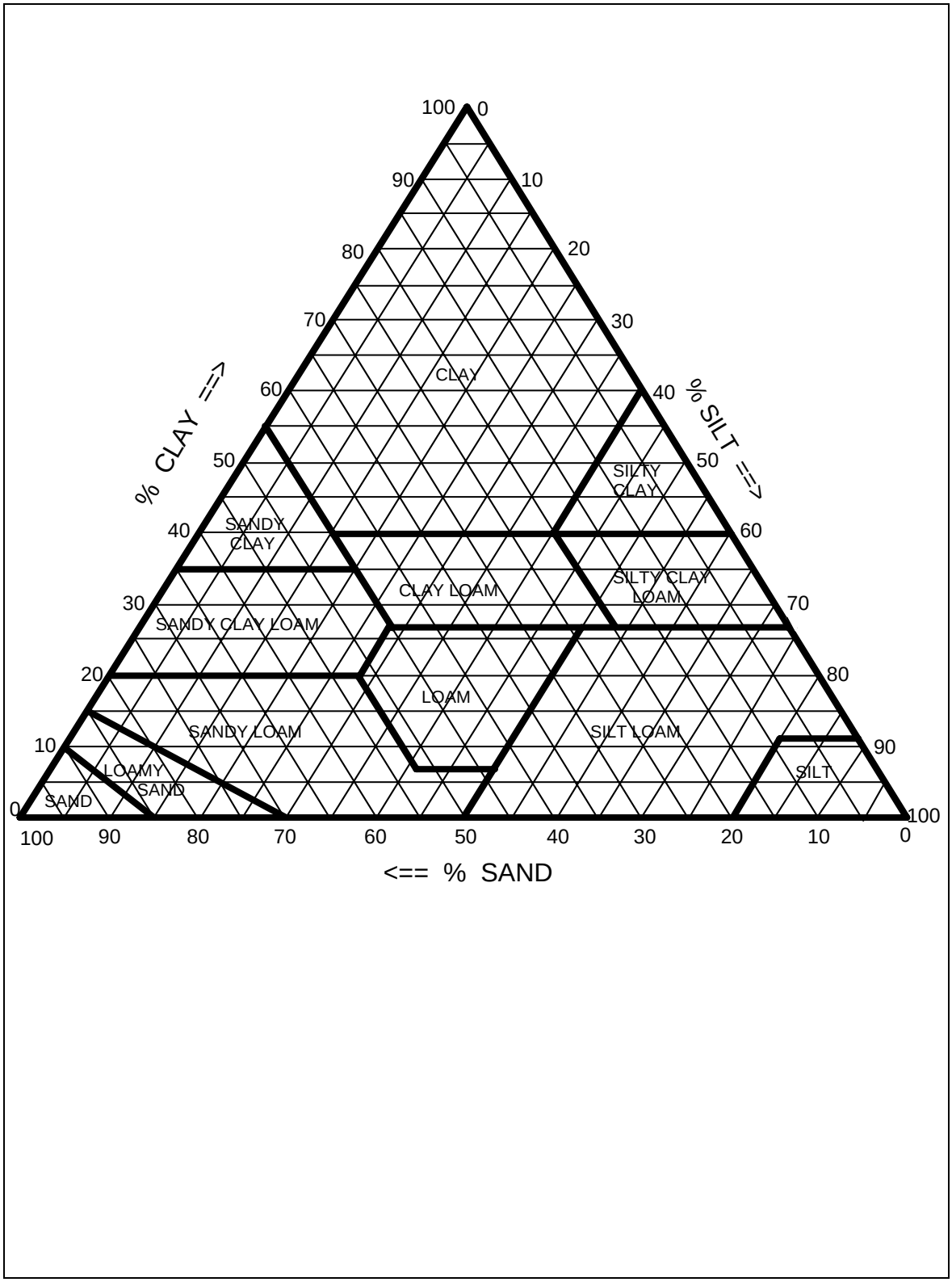
For the water referred to in Article 6(1)(a), (b) and (d), the value must be met, at the latest, 10 calendar years after the entry into force of this Directive. The parametric value for total THMs from five years after the entry into force of this Directive until 10 years after its entry into force is 150 µg/l.

Member States must ensure that all appropriate measures are taken to reduce the concentration of THMs in water intended for human consumption as much as possible during the period needed to achieve compliance with the parametric value.

When implementing the measures to achieve this value, Member States must progressively give priority to those areas where THM concentrations in water intended for human consumption are highest.

[35] To be added following the outcome of the study currently being carried out

Appendix 3: Soil classification



Textural classes of mineral soils according to the US soil classification. Particle sizes:

sand	>50 µm
silt	2 – 50 µm
clay	<2 µm

Appendix 4: Partition coefficients – glossary

This appendix gives a brief overview of terminology and equations used with respect to partition coefficients encountered in soil and sediment adsorption studies.

In the field of environmental chemistry and ecotoxicology, the distribution of a compound over two different environmental compartments is commonly described using an equilibrium constant, expressed by the capital letter *K*. The equilibrium constant describes a ratio of concentrations of a chemical compound in two different phases, similar to the description of the dissociation constant of acids and bases at equilibrium (usually pK_a).

Since the solute-solvent-sorbent system is assumed to be in thermodynamic equilibrium, *K* can be considered a constant; however, it is valid only for the conditions (pH, temperature, concentration range, type of sorbent, etc.) employed during its determination. To illustrate that the ratio refers to the *distribution* of a compound over two phases rather than a concentration ratio in identical phases, a subscript d (for distribution) is added: K_d.

The term *partitioning* is also used to describe the distribution of a compound over different phases, e.g. when describing the partitioning of a compound between octanol and water: K_{ow}. In practice, distribution constants of metals between water and soil (or sediment, or suspended matter) are often expressed as K_p values, and are then referred to as partition coefficients (rather than constants). In fact, both K_d and K_p are used here to describe the same process (i.e. adsorption) and can be seen as synonyms. In the pesticide registration framework, $K_{s/l}$ is also used to describe the same parameter and is called solid/liquid partition coefficient.

When sorption is independent of the concentration of the compound of interest, the sorption isotherm[36] is linear and K_d is calculated as follows:

$$K_d = K_p = \frac{C_s}{C_w} \qquad (69)$$

in which K_d and K_p are the linear distribution coefficient, linear partition coefficient or simply: linear sorption coefficient [L.kg^{-1}]
C_s is the concentration in the solid phase [mg.kg^{-1}]
C_w is the concentration in the aqueous phase [mg.L^{-1}]
The units presented are those most commonly encountered in scientific literature, but different units may also be used.

The relationship most often used to describe non-linear sorption is the (empirical) Freundlich model:

$$C_s = K_f \times C_w^{\frac{1}{n}} \qquad (70)$$

in which K_f is the Freundlich sorption coefficient [L.kg^{-1}]
n is an empirically determined parameter [-]

[36] A sorption isotherm is the relationship between the adsorbed concentration (dependent variable) and the dissolved concentration of a compound, determined at a constant temperature.

When $n = 1$, sorption is linear and $K_f = K_d$. When $n > 1$, the sorption isotherm is curved downward, with $n < 1$, the sorption isotherm is curved upward. It is not possible to specifically address the causes of non-linearity of sorption isotherms. Both compound properties and sorbent characteristics influence sorption behaviour and at present, no general agreement exists on the mechanism(s) of sorption (Ten Hulscher, 2005).

Linearity or non-linearity of sorption can be investigated by plotting logarithms of C_s versus logarithms of C_w. The slope of the linear function fitted through the data points is $^1/_n$ and the logarithmic form of 70 is a linear relationship when $n = 1$. In evaluating adsorption studies in the framework of Dutch pesticide registration, K_f values are considered acceptable when $^1/_n$ is within the range of 0.7 – 1.1 (Mensink *et al.*, 1995). We refer to Mensink *et al*. for quality criteria when reviewing batch adsorption studies.

K_f values are accepted as K_d values without correction when $^1/_n$ values are within the range of 0.7 – 1.1. K_f values with $^1/_n$ values outside the range of 0.7 – 1.1 are considered unreliable and are not used for ERL derivation.

For many organic compounds (in particular, neutral hydrophobic compounds), the sorption constant is directly proportional to the quantity of organic matter of the sorbent (Boethling and Mackay, 2000). K_p can then be normalised to the organic carbon content of the sorbent:

$$K_{oc} = \frac{K_p}{F_{oc}} \qquad (71)$$

in which K_{oc} is organic carbon normalised sorption coefficient [L.kg^{-1}]
Kp is the sorption coefficient [L.kg^{-1}]
F_{oc} is the fraction organic carbon of the sorbent [-]

When the percentage of organic carbon of the sorbent is not reported it can be calculated from the percentage organic matter using a conversion factor. In equation:

$$\%\,oc = \frac{\%\,om}{1.7} \qquad (72)$$

in which % oc is the percentage organic carbon of the sorbent [% (w/w)]
% om is the percentage organic matter of the sorbent [% (w/w)]
1.7 is a conversion factor [-]
For most soils, organic matter contains 1/1.7× 100% = 58.8% organic carbon.