

RIVM report 601501 012

**Guidance Document on deriving
Environmental Risk Limits**
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Abstract

This report is an update of previous guidance documents for deriving environmental risk limits in the Netherlands. The updated methodology to derive risk limits for water, groundwater, soil, sediment and air and their harmonisation is presented. The document covers the derivation of the Ecotoxicological Serious Risk Concentration (SRC_{ECO}), the Maximum Permissible Concentration (MPC) and the Negligible Concentration (NC).

Preface

This report is a result of the project ‘Setting Integrated Environmental Quality Standards’, with contact person dr. M. van der Weiden at the Ministry of Housing, Spatial Planning and the Environment (VROM-DGM./SAS). The contact person at RIVM is Dr. D. Sijm (CSR).

This report was discussed by the members of the “Environmental Quality Standards Advisory Group (abbr. OZBG-ECO)”, who are acknowledged for their contribution. The members are dr. T. Brock (Institute for Forestry and Nature Research), drs. S. Dogger (Health Council of the Netherlands), dr. J. Faber (Institute for Forestry and Nature Research), dr. K. den Haan (Shell International Chemical BV), Mrs. J. Pijnenburg (National Institute for Coastal and Marine Management), drs. M. Koene (Foundation for Nature and Environment), dr. D. Sijm (National Institute of Public Health and the Environment, secretary), dr. E. Sneller (National Institute of Inland Water Management), dr. J. Struijs (National Institute of Public Health and the Environment), drs. T.P. Traas ((National Institute of Public Health and the Environment), dr. J. Appelman (Board for the Authorisation of Pesticides), dr. W. van Tilborg (VTBC), dr. M. van der Weiden (Ministry of Housing, Spatial Planning and the Environment), and chaired by dr. J. van Wensem (Technical Soil Protection Committee).

More information on Environmental Risk Limits and Quality Standards can be found in a compilation of methodology and RIVM reports on this subject (De Bruijn et al., RIVM report 601640 001), in the book *Environmental Quality Standards in The Netherlands 1999* (Samson Publishers, Alphen aan de Rijn, The Netherlands) and on the website of the Centre for Substances and Risk Assessment, RIVM (<http://www.rivm.nl/csr/>).

Contents

SAMENVATTING	7
SUMMARY	8
1. INTRODUCTION	9
1.1 FOCUS AND AIM	9
1.2 READERS' GUIDE	9
2. OVERVIEW	11
2.1 PARTIES AND RESPONSIBILITIES	11
2.2 ERLs AND EQS IN THE NETHERLANDS	11
2.2.1 SRC _{ECO}	13
2.2.2 MPC	14
2.2.3 NC	15
3. DATA COLLECTION	17
3.1 SOURCES	17
3.2 LITERATURE SEARCH	18
3.3 REQUIRED DATA	18
3.3.1 Physico-chemical data	18
3.3.1.1 Water solubility	19
3.3.1.2 Henry's Law constant	19
3.3.1.3 n-Octanol/water partition coefficient (log K _{ow})	19
3.3.2 Data on fate and behaviour	20
3.3.2.1 Properties concerning degradation/metabolite formation	20
3.3.2.2 Partition coefficients	20
3.3.3 Toxicity data	23
3.3.3.1 Aquatic toxicity data	23
3.3.3.2 Terrestrial toxicity data	25
3.3.3.3 Sediment toxicity data	26
3.3.3.4 Air toxicity data	26
3.3.3.5 Secondary poisoning	26
4. DATA EVALUATION AND TREATMENT	29
4.1 RELIABILITY AND USEFULNESS OF STUDIES	29
4.2 FATE AND BEHAVIOUR	29
4.2.1 Partition coefficients	30
4.3 ECOTOXICOLOGICAL DATA	30
4.3.1 Preferred endpoints	30
4.3.2 Other endpoints	30
4.3.3 Test conditions	31
4.3.4 Test duration	32
4.4 DATA SELECTION AND TREATMENT	33
4.4.1 Aquatic toxicity data and general remarks	33
4.4.1.1 General calculations (all compartments)	33
4.4.1.2 Statistical analysis	34
4.4.2 Soil toxicity data	35
4.4.2.1 Recalculation to standard soil	35
4.4.3 Sediment toxicity data	37
4.4.4 Air toxicity data	37
4.4.5 Field studies	38
4.4.5.1 Aquatic field studies	38
4.4.5.2 Terrestrial field studies	38
4.4.6 Secondary poisoning	39
4.4.6.1 Bioconcentration factors	39
4.4.6.2 Biota to Sediment Accumulation Factors	41
4.4.6.3 Toxicity studies with birds and mammals	42
4.4.6.4 Conversion of bird and mammal NOECs	43
5. DATA TABLES	45

5.1	AQUATIC TOXICITY DATA.....	45
5.1.1	Species	45
5.1.2	Species properties	45
5.1.3	Analysis of test compound	46
5.1.4	Test type.....	46
5.1.5	Substance purity/compound	46
5.1.5.1	Substance purity.....	46
5.1.5.2	Test compound	46
5.1.6	Test water.....	46
5.1.7	pH.....	47
5.1.8	Water properties.....	47
5.1.8.1	Hardness	47
5.1.8.2	Salinity	47
5.1.9	Exposure time	47
5.1.10	Test criterion	48
5.1.11	Ecotoxicological endpoint.....	48
	Test result and derivation of L(E)C50/NOEC	48
5.1.11.1	L(E)C50 values.....	48
5.1.11.2	NOEC values.....	48
5.1.12	Notes	49
5.1.13	Reference	49
5.2	SOIL TOXICITY DATA	49
5.2.1	Species/process/activity	49
5.2.1.1	Microbial processes/enzyme activities.....	49
5.2.1.2	Species.....	49
5.2.2	Species properties	49
5.2.3	Soil type	50
5.2.4	pH.....	50
5.2.5	% organic matter (% OM).....	50
5.2.6	% clay.....	50
5.2.7	Temperature	50
5.2.8	Exposure time	50
5.2.9	Test criterion	51
5.2.10	Ecotoxicological Endpoint	51
5.2.11	Result test soil	51
5.2.12	Result standardised soil/sediment	52
5.2.13	Notes	52
5.2.14	Reference	52
5.3	BIRD AND MAMMAL TOXICITY DATA	53
5.3.1	Species	53
5.3.2	Species properties	53
5.3.3	Substance purity.....	53
5.3.4	Application route.....	53
5.3.5	Exposure time	53
5.3.6	Test criterion.	53
5.3.7	Ecotoxicological Endpoint	53
5.3.8	Effect concentration gavage	53
5.3.9	Effect concentration diet	54
5.3.10	Notes	54
5.3.11	Reference	54
5.4	PARTITION COEFFICIENTS	54
5.4.1	Test substance	54
5.4.2	Substance purity.....	54
5.4.3	Soil type	54
5.4.4	Organic carbon content	54
5.4.5	pH.....	54
5.4.6	Cation exchange capacity (CEC)	54
5.4.7	Solid/water mass distribution (g/l)	55
5.4.8	Mass balance	55
5.4.9	Equilibration time	55
5.4.10	Log K _{oc}	55

5.4.11	Notes	55
5.4.12	Reference	55
5.5	BCFs OR BSAFs	55
5.5.1	Species	55
5.5.2	Species properties	55
5.5.3	Test type.....	56
5.5.4	Substance purity	56
5.5.5	Test water	56
5.5.6	pH.....	56
5.5.7	Water properties.....	56
5.5.7.1	Hardness	56
5.5.7.2	Salinity.....	56
5.5.8	Exposure time	56
5.5.9	Exposure concentration.....	56
5.5.10	Time to Equilibrium.....	56
5.5.11	Dry to wet weight ratio	56
5.5.12	BCF/BSAF	56
5.5.13	Notes	57
5.5.14	Reference	57
5.6	ERLs.....	57
6.	CALCULATING ENVIRONMENTAL RISK LIMITS.....	59
6.1	REFINED EFFECT ASSESSMENT	59
6.1.1	Introduction.....	59
6.1.2	Deriving ERLs	61
6.2	PRELIMINARY EFFECT ASSESSMENT	62
6.2.1	TGD/EU factors	63
6.2.2	Modified EPA assessment factors.....	65
6.2.3	Deriving SRC _{ECO}	66
6.3	SECONDARY POISONING	67
6.4	THE ADDED RISK APPROACH	67
6.5	EQUILIBRIUM PARTITIONING METHOD.....	68
6.5.1	The modified equilibrium partitioning method.....	70
6.6	FINAL HARMONISATION OF ERLS.....	70
6.7	HUMAN-TOXICOLOGICAL RISK LIMITS AND INTEGRATION WITH ERLS FOR AIR.....	73
7.	CONCLUDING REMARKS	75
7.1	CURRENT ERLS AND EQSS.....	75
7.2	PERSPECTIVE	76
7.2.1	Statistical Issues	76
7.2.2	Bioavailability	77
7.2.3	Integration of human risk limits.....	77
7.2.4	Data limitations	77
	REFERENCES	79
	ANNEX 1A. TAXONOMIC POSITION OF SELECTED GROUPS OF AQUATIC SPECIES.....	87
	ANNEX 1B: TAXONOMIC POSITION OF SELECTED GROUPS OF SOIL SPECIES	88
	ANNEX 2. LITERATURE SEARCH PROFILES	89
	ANNEX 3A. AQUATIC TOXICITY DATA TABLES	91
	ANNEX 3B. SOIL TOXICITY DATA TABLES	92
	ANNEX 3C. EQUILIBRIUM PARTITION COEFFICIENT DATA TABLE	93
	ANNEX 3D. BIOCONCENTRATION FACTORS DATA TABLE	93
	ANNEX 3E. BIRD AND MAMMAL TOXICITY DATA TABLE.....	94
	ANNEX 4. AMERICAN SOIL CLASSIFICATION SYSTEM	95
	ANNEX 5. GLOSSARY	96
	ANNEX 6. EXTRAPOLATION FACTORS FOR ESTIMATING LOG HAZARDOUS CONCENTRATIONS	98
	ANNEX 7. PROBABILISTIC MODELING.....	99
	ANNEX 8. QSARS FOR AQUATIC TOXICITY OF CHEMICALS ACTING BY NARCOSIS	101
	ANNEX 9. DOCUMENTATION REQUIREMENTS	103
	ANNEX 10. CALCULATION OF ERLS FOR TOTAL WATER CONCENTRATIONS	106
	ANNEX 11: DERIVATION OF MPCs IN AIR FOR HUMANS AND HARMONISATION	108
	ANNEX 12: MAILING LIST.....	117

Samenvatting

Dit rapport is een revisie van voorgaande protocollen voor het afleiden van milieurisicogrenzen in Nederland (Slooff, 1992; Crommentuijn et al., 1994; Kalf et al., 1999). Dit document bestrijkt de dataverzameling, data-evaluatie en afleiding van de “Serious Risk Concentration” voor het ecosysteem (SRC_{ECO}), het Maximum Toelaatbaar Risico (MTR) en het Verwaarloosbaar Risico (VR). Deze Milieurisicogrenzen worden in principe afgeleid voor de milieucompartimenten zoetwater, zoutwater, lucht, bodem, sediment en grondwater, mits de aanwezige data dit toestaan. Richtlijnen worden gegeven voor het documenteren en rapporteren van de milieurisicogrenzen.

Twee methoden worden gebruikt om risiconiveaus te berekenen met behulp van ecotoxicologische studies:

De “refined effect assessment” volgens een herziene statistische extrapolatiemethode (Aldenberg & Jaworska 2000) en de “preliminary effect assessment” die gebruik maakt van assessment factoren van de “Technical Guidance Documents” (ECB, 1996). Als niet aan de eisen van de ECB kan worden voldaan, worden assessment factoren volgens de modified EPA method gebruikt (OECD, 1992). Het toepassen van de refined effect assessment met als invoer chronische toxiciteitsdata heeft de voorkeur. Deze methode wordt toegepast bij ten minste 4 chronische NOEC waarden voor 4 soorten uit verschillende taxonomische groepen. Indien deze dataset niet beschikbaar is, worden assessment factoren toegepast volgens de “preliminary effect assessment” method.

Milieurisiconiveaus voor bodem en sediment kunnen bij gebrek aan data ook indirect afgeleid worden uit de risiconiveaus voor water. Hierbij wordt gebruik gemaakt van de Equilibrium partitie theorie (EqP methode). Met deze methode wordt de concentratie in bodem of sediment berekend met behulp van partitiecoëfficiënten en is gebaseerd op de aanname dat er evenwicht bestaat tussen de stof in het (porie)water en de stof die is gebonden aan de bodem of het sediment.

Intercompartimentele uitwisselingsprocessen mogen niet leiden tot een overschrijding van risiconiveaus. Om dit te vermijden wordt de EqP methode toegepast om de risiconiveaus van de individuele compartimenten te harmoniseren.

Het concept van toegevoegd risico wordt gebruikt om rekening te houden met natuurlijke achtergrondconcentraties. Een berekende Maximum Toelaatbare Toevoeging (MTT) wordt opgeteld bij de achtergrondconcentratie; het MTR is dus de som van MTT en de achtergrondconcentratie.

Als de $\log K_{ow}$ groter dan 3 is, of een trage afbraak, biotransformatie of excretie wordt verwacht, worden aanvullende gegevens verzameld over bioaccumulatie in de voedselketen (doorvergiftiging). Risiconiveaus worden dan berekend gebaseerd op de mogelijkheid van doorvergiftiging, waarbij de afleiding op twee manieren plaatsvindt. Specifieke procedures zijn beschikbaar voor het afleiden van milieurisiconiveaus voor narcotische verbindingen, gebaseerd op QSARs en voor de afleiding van risiconiveaus voor vluchtige stoffen waarbij de lucht de dominante blootstellingsroute is.

Summary

This report is an update of previous guidance documents for deriving environmental risk limits (ERLs) in the Netherlands (Slooff, 1992; Crommentuijn et al., 1994; Kalf et al., 1999). This document covers data collection, data evaluation and derivation of the Serious Risk Concentration (SRC), the Maximum Permissible Concentration (MPC) and the Negligible Concentration (NC). These ERLs are in principle derived for the compartments fresh water, salt water, air, soil, sediment and groundwater, data permitting. Guidance is also provided for documentation and reporting of ERLs.

Two methods are used to derive ERLs from ecotoxicological studies: the refined effect assessment method with revised statistical extrapolation (Aldenberg and Jaworska, 2000) and the preliminary effect assessment method using assessment factors of the Technical Guidance Documents (ECB, 1996). In case the requirements of the ECB are not met, the modified EPA method is used (OECD, 1992). Since long-term chronic toxicity data are preferred, the aim is to apply the refined effect assessment method. This method can only be applied if at least four chronic NOEC values for four species from different taxonomic groups are available. If such a minimal data set is not available, preliminary effect assessment with assessment factors is applied.

ERLs for soil and sediment can also be derived indirectly from the ERL for water if experimental data are lacking, by using the equilibrium partitioning method (EqP-method). This method estimates the concentration in the soil or sediment using partition coefficients and is based on the assumption that equilibrium exists between the chemical sorbed to the solid phase and the pore water.

To account for intercompartmental exchange processes that might occur if disequilibrium exists, the EqP-method is used to harmonise the ERLs of the individual environmental compartments.

The added risk approach is used to take natural background concentrations into account when calculating MPCs for naturally occurring substances: a maximum permissible addition (MPA) is calculated from laboratory toxicity tests. This MPA is considered to be the maximum concentration that can be added to the background concentration (C_b), without causing deleterious effects. Hence, the MPC is the sum of the C_b and the MPA.

If $\text{Log } K_{ow} > 3$ or low degradation or high accumulation rates are expected, additional data on secondary poisoning are needed. In this case, ERLs are calculated based on the accumulation potential of a compound in top predators, for which two methods are available that are compared. Specific procedures are available for the derivation of ERLs for narcotic substances, based on QSAR estimates of toxicity, and for derivation of harmonised ERLs for volatile substances (where air is the dominant exposure route).

1. Introduction

1.1 Focus and aim

Environmental risk limits (ERLs) have been derived for a large number of substances (e.g. Crommentuijn et al., 2000a,b) and serve as advisory values to set environmental quality standards (EQS) by the government for various policy purposes. The term EQS is used to designate all legally and non-legally binding standards that are used in Dutch environmental policy. EQSs are used to (VROM, 1998):

- Systematically evaluate the environmental quality with national, regional and local monitoring programs that measure the concentration of substances in the environment.
- Develop source-orientated policy and policy to further reduce and control emissions to meet the general basis of the overall environmental policy, which is sustainable development (VROM, 1989a; VROM, 1994). Sustainable development means that the quality of the environment is guaranteed for the next generation and beyond: exposure to substances should not result in 'adverse' effects on man and ecosystems
- Judge the necessity of legally binding EQSs
- Derive EQSs for products and agro-chemicals
- Evaluate and develop goals and targets for specific socio-economic parties (target groups)
- Evaluate and develop goals for regional and national government authorities
- Grant licenses and permits concerning environmental quality.

The methods to derive environmental risk limits (ERLs) in the Netherlands are described in two documents (Slooff, 1992 and Crommentuijn et al., 1994).

These protocols have been used to derive risk limits for a large number of substances (e.g. Crommentuijn et al., 2000a,b). De Bruijn et al. (1999) have compiled the entire procedure and results up to 1997. Experience has led to a number of changes, improvements and extensions of the protocols that have been published in various documents (e.g. Kalf et al., 1999; Smit et al., 2000; Verbruggen et al., 2000). The present guidance document is an update of the previous ones and includes the changes up to December 2000. It provides guidance on the methodology of deriving environmental risk limits. It reflects the current procedure for deriving ERLs by RIVM. Minimum requirements for data search, data analysis and documentation of ERLs are formulated. Other certified parties (e.g., RIKZ and RIZA, see glossary) can also derive ERLs according to the procedure in this document.

1.2 Readers' guide

The structure of the report is based on the chronological steps needed for deriving ERLs. Chapter 2 provides an overview of the context and the procedures of deriving ERLs for those unfamiliar with the methodology. Chapter 3 deals with literature search and data requirements. The evaluation of ecotoxicological studies is outlined in

Chapter 4. Chapter 5 describes the format that is used at RIVM for tabulating the data. Furthermore, specific details about documenting studies and recalculations are mentioned for several evaluation criteria. Chapter 6 concerns the methods used for deriving ERLs: refined effect assessment, preliminary effect assessment, the method to incorporate secondary poisoning in MPC derivation, the added risk approach, the equilibrium partitioning method and final harmonisation of ERLs. Chapter 7 ends with concluding remarks.

2. Overview

2.1 Parties and responsibilities

The ministry of VROM developed the current framework in which the responsibilities concerning the derivation of ERLs are laid down. The methodology for deriving scientifically underpinned ERLs is the responsibility of the Centre for Substances and Risk assessment (CSR) of the National Institute of Public Health and Environmental Protection (RIVM). The methodology for deriving ERLs has to be agreed upon by an inter-departmental Steering Group for standard setting (in Dutch: Stuurgroep INS) and the Dutch Board for the Authorisation of Pesticides (in Dutch: commissie toelating bestrijdingsmiddelen, CTB). ERLs can in principle also be derived in the framework of the admission of plant protection products and biocides (In Dutch: 'Besluit Milieutoelatingseisen Bestrijdingsmiddelen'). The responsibility for this task is delegated to the Dutch Board for the Authorisation of Pesticides. The procedure for deriving ERLs for plant protection products and biocides is harmonised with the general protocol for deriving ERLs (Kalf et al., 1999). The Steering Group 'Pesticide Policy' (in Dutch: Stuurgroep Bestrijdingsmiddelenbeleid) should also ratify the methodology for deriving ERLs.

Other certified parties such as the Institute for Inland Water Management and Wastewater Treatment (RIZA) and the Institute for Coast and Sea (RIKZ) can also derive ERLs. Subcontracting third parties can derive ERLs for pesticides by commission of the CTB. Any party should derive ERLs according to the procedures laid down in this guidance document. ERLs always need to be verified by the Environmental Quality Standards Advisory Group (in Dutch: Onderzoeks-begeleidingsgroep-ecotoxicologische risico's), independent of the framework in which they are derived. Risk Limits that are used for admission policy of plant protection products and biocides that deviate from the protocol in this guidance document are not ERLs as defined in this guidance document¹.

ERLs are used as scientific advisory values to set Environmental Quality Standards (EQS) by the government. Table 1 shows the relationship between the different ERL and EQS. The government can take into consideration the advice of consulting parties, such as the Dutch Health Council (in Dutch: Gezondheidsraad, GR) or the Dutch Technical Soil Protection Committee (in Dutch: Technische Commissie Bodembescherming, TCB), when setting the EQS. In addition, when setting the Intervention Value additional socio-economic factors can be taken into account.

2.2 ERLs and EQS in The Netherlands

ERLs are derived for different environmental compartments, based on observed or expected effects on species inhabiting these compartments, including effects from food chain exposure of predators (secondary poisoning).

¹ Risk limits derived for admission policy can take into account specific studies such as microcosm studies or semi-field experiments (higher tier testing). The relation between generic ERLs (this document) and limits derived for admission policy is not yet decided.

Table 1. Environmental Risk Limits (ERLs) and the related Environmental Quality Standards (EQS) that are set by the Dutch government in The Netherlands for the protection of ecosystems.

NC Negligible Concentration

MPC Maximum Permissible Concentration

SRC_{eco} Serious Risk Concentration for the ecosystem

Description	ERL	EQS
The NC represents a value causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account possible combined effects.	NC (for air, water, soil, groundwater and sediment)	Target Value (for air, water, soil, groundwater and sediment)
A concentration of a substance in air, water, soil or sediment that should protect all species in ecosystems from adverse effects of that substance. A cut-off value is set at the fifth percentile if a species sensitivity distribution of NOECs is used. This is the Hazardous Concentration for 5% of the species, the HC_5^{NOEC} .	MPC (for air, water, soil, groundwater and sediment)	MPC (for air, water, sediment and air)
A concentration of a substance in the soil, sediment or groundwater at which functions in these compartments will be seriously affected or are threatened to be negatively affected. This is assumed to occur when 50% of the species and/or 50% of the microbial and enzymatic processes are possibly affected.	SRC _{eco} (for water, soil, groundwater and sediment)	Intervention Value (for soil, sediment and groundwater)

ERLs are derived using single-species toxicity data or processes for soil and physico-chemical characteristics, with different approaches depending on the amount of information available. When chronic toxicity data for 4 or more species of at least 4 different taxonomic groups (Annex 1) are available for a particular environmental compartment, a statistical procedure is applied to derive ERLs (Refined effect assessment, Section 6.1). When less data is available a set of assessment factors are applied, varying from 10 to 1000, depending on the type of data (Preliminary effect assessment, Section 6.2).

If toxicity data for species representative of soil or sediment cannot be found or are insufficient, equilibrium partitioning (Di Toro et al., 1991) is applied to derive ERLs for soil or sediment from the ERL for water. In that case, soil/water or sediment/water partition coefficients are required. This procedure is elaborated in Sections 3.3.2, 4.2.1 and 6.5.

The various ERLs are:

- the Negligible Concentration (NC) for water, soil, groundwater, sediment and air
- the Maximum Permissible Concentration (MPC) for water, soil, groundwater sediment and air
- the Ecotoxicological Serious Risk Concentration for water, soil, groundwater and sediment (SRC_{ECO}).

ERLs for soil and sediment are calculated for a standardised soil (cf. section 4.4).

ERLs for water are reported for dissolved and total concentrations (including a standard amount of suspended matter) and if found significantly different, differentiated to freshwater and saltwater (cf. Section 4.4.1, Annex 10).

Each of the ERLs and its corresponding EQS represents a different level of protection, with increasing numerical values in the order Target Value < MPC^1 < Intervention Value. The EQS demand different actions when one of them is exceeded, explained elsewhere (VROM, 1994).

The EQS's Target Value and MPC are based on the NC and the MPC, respectively.

The Target Value is based only on ecotoxicological data. For soil, there is no EQS at the level of the MPC^2 . The Intervention Values for soil, groundwater and sediment are based on the lowest value of two underlying ERLs (Figure 1): one based on ecotoxicological data, the other based on human toxicological data and a human exposure model (Swartjes, 1999).

2.2.1 SRC_{ECO}

The SRC_{ECO} represents a level in the soil, sediment, water and groundwater at which functions in these compartments will be seriously affected or are threatened to be negatively affected. It is assumed that adverse effects on both ecotoxicological functioning and the structure of a ecosystem occur when 50% of the species and/or 50% of the microbial and enzymatic processes are possibly affected (Denneman and van Gestel, 1990). The Intervention value for soil can be based on serious risks for the soil ecosystem but can also be determined by other adverse effects such as on human health (VROM, 1990; cf. section 6.7).

The SRC_{ECO} for soil is derived in the project 'Risk related to soil quality'. A schematic outline of the procedure to derive the Intervention Value for soil and groundwater is presented in Figure 1. To account for intercompartmental exchange processes that might occur if dis-equilibrium would exist, harmonisation of SRC_{ECO} by Equilibrium partitioning is included (Di Toro et al., 1991).

¹ A complicating factor is that the term MPC is used both as an ERL and as an EQS. For historical reasons, however, the same abbreviation is used.

² Since the policy-related MPC is a level that needs to be aimed at in the short-term the MPC is considered to be less relevant for soil being a static compartment where a dilution of the substance or a reduction in the concentration of the substance is not to be expected in the short-term.

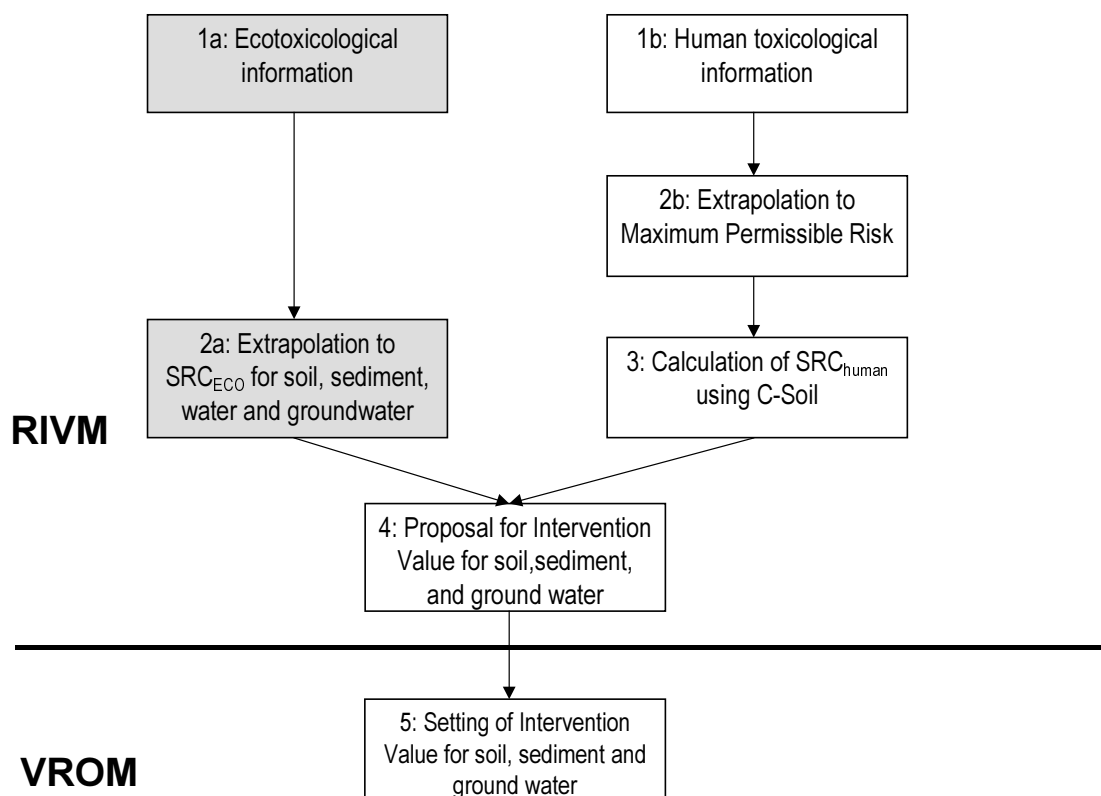


Figure 1: Diagram of the procedure to derive the Intervention value for soil and sediment clean-up (or remediation) and ground water remediation. The methodology used in the shaded boxes as outlined in this document is developed by the National Institute of Public Health and the Environment (RIVM). (Above the line), the Intervention Value is set by the Ministry of Housing, Spatial Planning and the Environment (VROM) (Below the line). SRC_{ECO} is the Ecotoxicological Serious Risk Concentration, SRC_{HUMAN} is the Human-toxicological Serious Risk Concentration, and C-Soil is a software program to calculate the SRC_{HUMAN} based on human exposure.

2.2.2 MPC

The MPC is set at a level that should protect all species in ecosystems from adverse effects of a substance (VROM, 1990). Pragmatically, a cut-off value is set at the fifth percentile if a species sensitivity distribution of NOECs is used in the refined effect assessment (Section 6.1). This is the Hazardous Concentration for 5% of the species, the HC_5^{NOEC} (Van de Meent et al., 1990; Aldenberg and Jaworska, 2000).

A schematic outline of the procedure to derive the MPCs is presented in Figure 2. MPCs are determined for the individual compartments water, soil, and sediment. Harmonisation of MPCs by Equilibrium Partitioning, to account for intercompartmental exchange processes that might occur if dis-equilibrium would exist, is included as well (Di Toro et al., 1991). MPCs for water, sediment and soil are derived in the project 'Setting Integrated Environmental Quality Standards'.

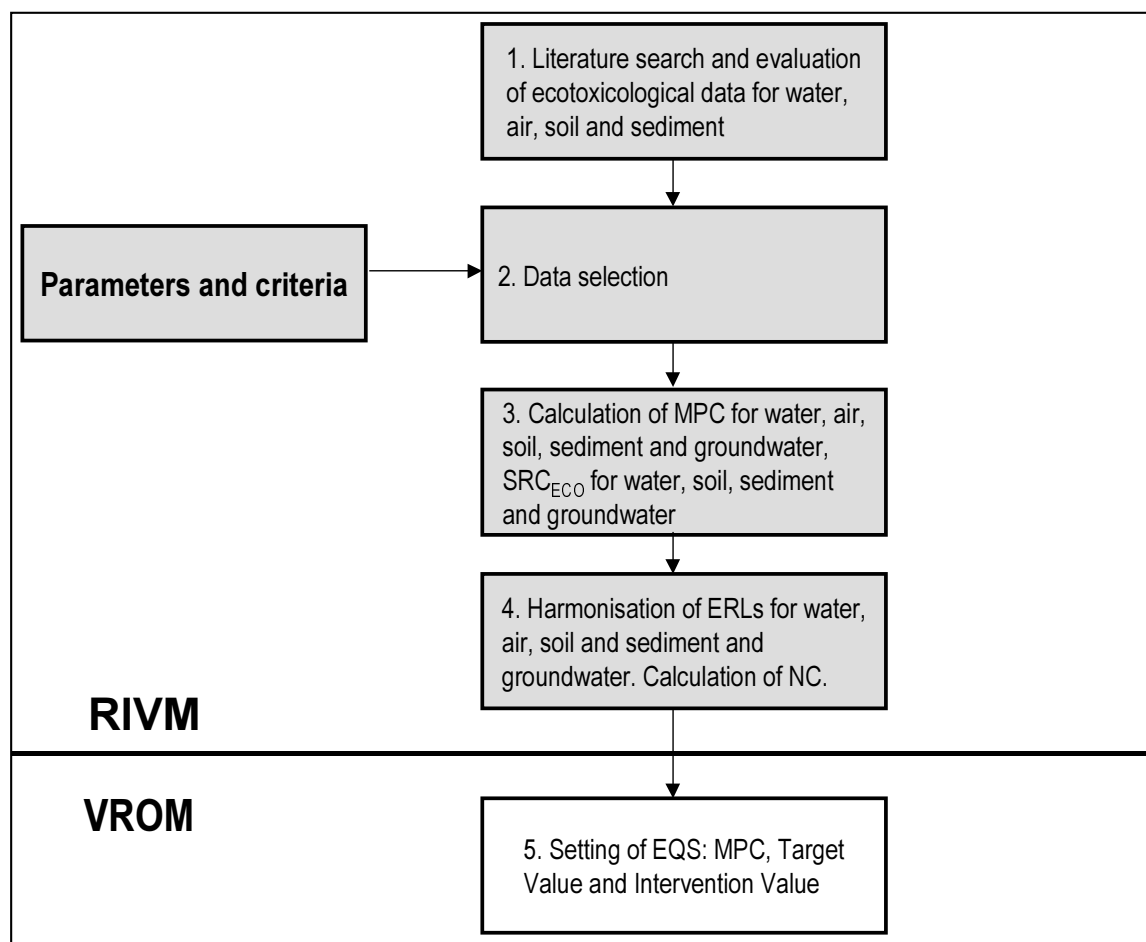


Figure 2: Diagram of the procedure to derive the Maximum Permissible Concentration (MPC) and the Target Value. The methodology used in the shaded boxes is outlined in this document. Above the dashed line the method to derive ERLs is indicated, i.e. MPC, NC and SRC_{ECO}, as documented by the National Institute of Public Health and the Environment (RIVM). Below the dashed line the MPC and Target Value is indicated, set by the Ministry of Housing, Spatial Planning and the Environment (VROM).

2.2.3 NC

The NC represents a value causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account the possible combined effects of the many substances encountered in the environment (Könemann, 1981; Deneer et al., 1988; VROM, 1989b). NCs are derived for the environmental compartments water, sediment, soil and air. The methodology to derive ERLs includes 4 steps. All steps are followed for a substance or a group of substances to calculate the MPC and NC for water, sediment, soil and air (Figure 2). The next chapters are concerned with the different steps.

3. Data collection

This chapter outlines the collection and evaluation of basic toxicity data for deriving ERLs. The basic data input for deriving ERLs is toxicity data for single-species or processes, sourced from the open primary literature. Basic data requirements for systematic data collection and compatibility are formulated. Additional data are to be collected if the substance has the potential to bioaccumulate through the food chain (secondary poisoning, Section 3.3.3.5 and 4.4.6). If no data are available at all, QSARs can be used as an alternative, but less reliable source of information.

3.1 Sources

The sources of literature that need to be consulted for collecting physico-chemical and ecotoxicological data depend on whether the substance is a plant protection product/biocide or not. For plant protection products and biocides, an admission dossier (containing confidential studies compulsory for admission and additional public literature) is received from the CTB (the confidential studies are found in application form A of the CTB (1995)). Existing monographs prepared by CTB or EU are considered of equal value. ERLs will be derived weighing all relevant data. The data search strategy should be reported in the methods of the final report. For compounds other than plant protection products and biocides the data set is formed almost entirely by public literature. In addition to public literature, involved parties (e.g. industry) are invited to submit relevant studies which will be treated as public literature.

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

- On-line search in Current Contents and Toxline (as available through Winspirls) using chemical name and or CAS number.
- On-line search in the bibliographic databases Biosis (ecotoxicological data and partition coefficients), TOXLINE (for mammalian data) and Chemical Abstracts (data on partition coefficients). The lay out of the search profiles is developed to use the host "Deutsches Institut für Medizinische Dokumentation und Information" (DIMDI), except for Chemical Abstracts for which the host DIALOG is used (see Annex 2).
- Libraries such as: the library of the Centre for Substances and Risk Assessment, the National Institute of Public Health and the Environment and the CTB library. Grey literature can be searched for depending on time and budget.
- The Internal literature database at RIVM is checked for relevant articles that already have been collected and evaluated.
- Confidential data from summaries evaluated in the 'Catch up Operation Pesticides I; Pandora's box' (Canton et al., 1991; Linders et al., 1994), or summarized in an 'Environmental Synopsis' are allowed to be used for derivation of ERLs only if these summaries have been accepted by the CTB. The studies described in these summaries are classified on the basis of quality indices (cf. section 4.1). Studies derived from CSR-summaries (e.g. pesticide studies) will not be evaluated again, with the exception of data used for calculation of the ERLs. In this case the

original study, available on microfilm, has to be re-evaluated. Data qualified with the reliability index 1 or 2 (see Section 4.1) are included, the reliability index 2 being mentioned in the footnote of the toxicity tables (see appendices). Data from studies with a reliability index 3 are handled as being not reliable and are not included.

- All secondary literature found will be used to find primary toxicity literature (retrospective literature search). The aim is to be as complete as possible. In principle *only primary literature* is used for MPC derivation (i.e.: original sources).

3.2 Literature search

The on-line search in the context of deriving ERLs is based on the year of publication of the most recent 'reliable' review. Whether or not a review is reliable, is based on expert judgement on a case-by-case basis. If no review is available it is advised to start the search from 1970 or from the beginning of the database in question. Based on expert judgement, other starting points can be used as well. Search profiles can be found in Annex 2.

3.3 Required data

Basic toxicity data are collected, tabulated according to a specific format (Annex 3) and reported (Annex 9). Basic physico-chemical data are needed for further reference, such as CAS numbers and the n-octanol/water partition coefficient (Section 3.3.1).

3.3.1 Physico-chemical data

Basic physico-chemical data should be collected and reported: IUPAC Name, CAS number, EINECS number, Structural formula (diagram), Empirical formula, Molar Mass, n-Octanol/water partition coefficient, Solubility, Melting Point, Vapour Pressure, Henry's law constant, pK values (dissociation constant) (cf. Annex 9.4.1). The following physical/chemical properties are especially important for deriving ERLs:

- Water solubility and melting point
- Henry's law constant and vapour pressure
- Octanol/water partition coefficients ($\text{Log } K_{ow}$).
- Solid/water partition coefficients (K_p)
- Degradation: hydrolysis, photolysis and biodegradation

Reliable sources for empirical or estimated physico-chemical properties of chemicals are the EpiWin database (SRC, 1997), the physical-chemical properties and environmental fate handbooks of Mackay et al. (1992-1997, compiled in Mackay et al. 1999), Boethling and Mackay (2000), or the MEDCHEM database (1992).

3.3.1.1 Water solubility

The water solubility is used to judge the reliability of a study. The water solubility is also used for calculation of the Henry's Law constant. The water solubility has to be determined at a temperature close to the temperature of the toxicity test, usually at 25 °C. Exceeding the water solubility is mentioned in a footnote to the toxicity data table: 'above water solubility, which is mg/l, temp. ...°C'. Studies in which results up to 10 times¹ above the water solubility are given, are considered to be acceptable for reporting in the tables. Results more than 10 times above the water solubility are not included. To facilitate dissolution of substances in water, carrier solvents are often used. Emulsifiers are not acceptable.

3.3.1.2 Henry's Law constant

To assess the volatilization of a compound from water the Henry coefficient (H) is used. Measured Henry's law constants, derived independently from toxicity tests, are preferred. The dimensionless Henry's law constant is calculated as:

$$H = \frac{P \cdot M}{S \cdot R \cdot T} \quad (1)$$

with P = vapour pressure in Pa,
 M = molecular weight in g.mol⁻¹,
 S = water solubility in g.m⁻³,
 R = 8.314 Pa.m³.mol⁻¹.K⁻¹,
 T = temperature in K.

In (semi)static tests with highly volatile substances it is difficult to maintain stable concentrations. Special attention is paid to the test conditions if $H > 3 \cdot 10^{-2}$ for the dimensionless Henry's Law constant (Lyman, 1981). If the mentioned limit is exceeded the test vessels must preferably be closed and be without headspace, or the concentration is measured and reported. This should be noted in the table. Also is reported whether the test vessels are aerated. If the test vessels in (semi)static tests are closed, special attention is paid to the oxygen concentration (for minimal permissible oxygen concentration: see OECD 1996).

3.3.1.3 n-Octanol/water partition coefficient (log K_{ow})

The log K_{ow} of a substance is used for:

- the estimation of aquatic toxicity with QSAR's
- estimation of BCF values
- cut off-value to assess the risk for secondary poisoning
- estimation of the organic carbon-water partitioning coefficient K_{oc}, when experimental data for K_{oc} are lacking

Experimental values obtained by the slow-stirring method are considered most reliable (De Bruijn et al., 1989). The log K_{ow} is derived from the MEDCHEM database; the star values from this database (MlogP) are preferred. If the star values are not available, the calculated value using the ClogP method is used which is also given in the MEDCHEM database. Verhaar and Hermens (1990) conclude that the ClogP estimation routine normally leads to reasonable values.

¹ An arbitrary cut-off value

3.3.2 Data on fate and behaviour

3.3.2.1 Properties concerning degradation/metabolite formation

A survey of hydrolysis, photolysis and biodegradation of the test substance is obligatory. Once it is established that hydrolysis and/or biodegradation is the (main) cause for an observed high loss, the question is if the metabolite(s) should have been tested instead of the parent compound, or if testing of both parent compound and metabolite(s) is necessary. The criteria of Whitehouse and Mallet (1993) are used for this decision, slightly changed by Mensink et al. (1995) (Table 2).

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

DT ₅₀	Selection
24 h	test is started with the parent substance
<4 h	test is started with metabolites
4-24 h	expert judgement

If a compound has a hydrolysis half-life of less than 4 hours the toxicity is based on the metabolites. No MPC for the initial compound can be derived. If the formed metabolites are stable an MPC can be derived for the main metabolites.

Toxicity studies (especially chronic) should always be checked for loss rates of chemicals. The renewal rate of the test medium should be in accordance with the (estimated) DT50. If the DT50 < renewal interval, the test is not acceptable.

3.3.2.2 Partition coefficients

Partition coefficients (K_p) are used when toxicity data for specific compartments are lacking and when ERLs are harmonised across compartments. K_p values can be acquired from experimental studies (as in pesticide registration), from databases or handbooks or, when other sources are lacking, estimated from K_{ow} using regressions. Data are tabulated according to Annex 3C.

3.3.2.2.1 Experimental studies

Sorption coefficients (K_p) are preferably derived from batch experiment studies. Batch experiments involve the shaking of soil, sediment or particulate matter with an aqueous solution containing the adsorbing chemical. The partition coefficient is calculated from:

$$K_p = \frac{C_s}{C_w} \quad (2)$$

with K_p = the solids-water partition coefficient [l/kg]
 C_s = the concentration in the solid phase [mg/kg]
 C_w = aqueous equilibrium concentration [mg/l]

For chemicals with a large affinity to the “third phase” (colloids and organic macromolecules that cannot be separated from the water phase) this method will lead to overestimation of the aqueous concentration and an underestimation of the K_p . Studies with calculation of a mass balance are preferred.

Sometimes experimental data are presented as a Freundlich adsorption isotherm. To derive an adsorption isotherm, the adsorbed fraction is measured for at least 4 to 5 initial concentrations. Within the scope of pesticide registration, K_f values are only selected if the Freundlich exponent ($1/n$) is within the range of 0.7 - 1.1 (Mensink et al., 1995):

$$C_s = K_f \cdot C_w^{1/n} \quad (3)$$

with C_s = the concentration in the solid phase [mg.kg^{-1}]
 K_f = the Freundlich constant [$\text{mg}^{(1-1/n)} \cdot \text{l}^{1/n} \cdot \text{kg}^{-1}$]
 C_w = the aqueous equilibrium concentration [mg.l^{-1}]
 $1/n$ = dimensionless exponent

To derive K_p 's from data reported in the form of Freundlich isotherms the following approach is chosen: with the parameters of the isotherm reported, the K_p is calculated using concentrations in water and soil at the lowest initial concentration used in the experiments and the following formula:

$$K_p = K_f \cdot \frac{C_w^{1/n}}{C_w} \quad (4)$$

with K_p = the soil-water partition coefficient [l.kg^{-1}]
 K_f = the Freundlich constant [$\text{mg}^{(1-1/n)} \cdot \text{l}^{1/n} \cdot \text{kg}^{-1}$]
 C_w = the aqueous equilibrium concentration [mg.l^{-1}]
 $1/n$ = dimensionless exponent

The organic carbon normalized partition coefficient (K_{oc}) can be calculated, if the fraction organic carbon f_{oc} is available, as:

$$K_{oc} = \frac{K_p}{f_{oc}} \quad (5)$$

with K_{oc} = organic carbon normalized soil-water partition coefficient [l/kg]
 K_p = soil-water partition coefficient [l/kg] for particular soil
 f_{oc} = fraction organic carbon of the soil (% organic carbon / 100)

Table 3 provides the information on relevant experimental conditions and results that are required for evaluating sorption coefficients, both for sediment/water and soil/water sorption coefficients.

Only studies in which the humus or organic matter content or organic carbon content is reported are accepted. Organic carbon content [$\text{g OC} / \text{g dw}$] is derived from the organic matter content [$\text{g OM} / \text{g dw}$] by dividing it by a conversion factor [$\text{g OM} / \text{g OC}$]:

$$OC = \frac{OM}{1.7} \quad (6)$$

Table 3. Information on relevant experimental conditions and results that are collected for equilibrium partition coefficients, i.e. both for soil/water and sediment/water partition coefficients. The underlined parameters are required.

Conditions	Parameters
Substance	<ul style="list-style-type: none"> • <u>Purity</u> (e.g. analytical grade or in percentage) • Organic carbon normalised sorption coefficient (K_{oc}) • <u>Added concentration corrected for background?</u> • Substance added in solution? • Check for mass balance
Soil	<ul style="list-style-type: none"> • Type of soil according to American soil type classification, and sample depth • <u>Soil characteristics</u> (organic matter content, pH, CEC)
Test conditions	<ul style="list-style-type: none"> • Is substance <u>analysed</u>? • <u>Soil to water ratio</u> • <u>Equilibration</u> time, before adding the test substance • <u>Duration</u> of the test (hours, days or months)
Results	<ul style="list-style-type: none"> • <u>Log K_{oc}</u> (for organic substances) • <u>Log K_p</u> (for metals and metalloids) • <u>Reference</u> of the study

The use of K_{oc}-values for metals and metalloids is not appropriate, and therefore, empirically derived K_p-values are selected. Empirical soil/water (K_{p,soil}) and sediment/water (K_{p,sed}) partition or distribution coefficients are used which most realistically mimic distribution processes in the Dutch environment.

3.3.2.2.2 Estimation of K_{oc} from K_{ow}

When experimental data are lacking, K_{oc}-values are collected from the SRC database or from handbooks (e.g. Mackay et al. (1999)). If a K_{oc} is unavailable, it can be estimated from K_{ow}, see below. The preferred equation, based on the precision of the QSAR, is chosen by expert judgement.

To derive log K_{oc}-values from log K_{ow}-values the QSAR regression equations of Gerstl (1990) should be used. If a specific group is not represented, an alternative source of QSARs can be used (Sabljic et al. 1995). Gerstl (1990) derived regression equations as given in formula for compounds from 16 chemical groups, based on a large database:

$$\log K_{oc} = a \log K_{ow} + b \quad (7)$$

with: K_{oc} = organic carbon normalized partition coefficient
K_{ow} = octanol-water partition coefficient
a and b = constants

These equations relating K_{ow} and K_{oc} are presented in Table 4.

Table 4: Regression parameters for estimation of $\log K_{oc}$

Group	a	b
All compounds	0.679	0.663
1 Acetanilides	-	-
2 Carbamates	0.433	0.919
3 Dinitroanilines	0.431	1.787
4 Aromatic hydrocarbons halogenated	0.722	0.417
5 Organophosphorous pesticides	0.689	0.530
6 Ureas	0.545	0.943
7 Triazines	0.586	0.826
8 Triazoles	0.583	0.969
9 Acids	-	-
10 PAH	0.762	1.051
11 Non-aromatic hydrocarbons halogenated	0.827	-0.039
12 Aromatic hydrocarbons non-halogenated	0.529	0.916
13 Amides	0.253	1.776
14 Phthalate esters	-	-
15 Organotin compounds	-	-
16 Miscellaneous	0.556	0.863

Some organic compounds contain acidic groups (e.g. hydroxyl or carboxyl groups) from which a proton can dissociate, leading to less hydrophobic negatively charged ions. A pH dependent partition coefficient can be calculated from the K_{ow} and the pK_a (Van de Meent et al. 1990). It appeared that these underestimated adsorption. Therefore, equation 8 (DiToro et al., 1991) is used for such compounds if no experimental values are available:

$$\log K_{oc} = \log K_{ow} [l/kg_{oc}] \quad (8)$$

3.3.3 Toxicity data

3.3.3.1 Aquatic toxicity data

Toxicity data that fulfill the minimum data requirements (Table 5) are evaluated (Chapter 4) and tabulated (Chapter 5, Annex 3A) in a specific format for later reference. This section outlines the requirements for toxicity data. If toxicity data are truly absent, QSAR estimates for aquatic toxicity are employed, see Annex 8. When sufficient data are absent, the \geq values may be used for evaluating tests that could not establish effective concentrations, and are the only available studies (see Section 4.4.1). Data tables are reported (Annex 9).

3.3.3.1.1 Direct route

For water, chronic and acute toxicity data are searched for and tabulated. An inventory is made of all the chronic toxicity data. When reliable chronic toxicity data are available for species from at least 4 taxonomic groups (Okkerman et al., 1993), a short but not exhaustive overview of the acute toxicity data is made. When reliable chronic toxicity data are available for species from less than 4 taxonomic groups, all literature on acute toxicity is evaluated. Toxicity data are collected for both freshwater

and marine species. A statistical evaluation is performed to determine whether freshwater and saltwater have to be treated separately or can be combined (Section 4.4.1).

Table 5 provides the information on relevant experimental conditions and results that are collected and required for aquatic species.

Table 5. Information on relevant experimental conditions and results that are collected for chronic toxicity studies on aquatic species. The underlined parameters are required.

Conditions	Parameters
Organism	• <u>Species</u> , taxon, strain, scientific name, <u>age</u> , <u>weight</u> , <u>size</u> and <u>life stage</u>
Substance	• <u>Purity</u> (e.g. analytical grade or in percentage)
Test water	• Natural water, tap water, reconstituted water, artificial medium
Test conditions	<ul style="list-style-type: none"> • Is substance <u>analysed</u> or is endpoint based on <u>nominal</u> concentration? • Flow-through, static or semi-static experiment, etc. • <u>Duration</u> of the test (hours, days or months) • <u>Type of endpoint</u> (growth, reproduction, mobility, mortality)
Results	<ul style="list-style-type: none"> • <u>Expression of endpoint</u> (LCx, ECx, NOEC, etc.) • <u>Reference</u> of the study

3.3.3.1.2 Insufficient data

When no or only few toxicity data are available, and the substance is exerting its toxicity via a non-specific mode of action (Verhaar et al., 1992), QSARs are used to estimate aqueous toxicity. The QSARs are based on the correlation between the toxicity of a certain compound and one or more structural parameters of the compound (e.g. log K_{ow}), normally through uni- or multivariate linear regression or sometimes through nonlinear regression (Verhaar et al., 1992).

QSARs can only be established for compounds with a common mode of toxic action. Six modes of action are distinguished: nonpolar narcosis, polar narcosis, uncoupling of oxidative phosphorylation, respiratory membrane irritation, acetylcholinesterase inhibition and central nervous system seizure (McKim et al., 1987; Bradbury et al., 1989). The mechanism of narcosis is non-specific: the potency of a chemical to induce narcosis is entirely dependent on its hydrophobicity. This implies that, in the absence of all specific mechanisms of toxicity, a chemical will always be as toxic as its hydrophobicity (e.g. log K_{ow}) indicates, or in other words, no chemical will be less toxic than implied by its hydrophobicity. Narcosis type toxicity is therefore also called “baseline” toxicity or minimum toxicity. Structural requirements for chemicals acting through narcosis have been described by Verhaar et al. (1992).

For the category of substances with a non-specific mode of action the QSARs are determined on the basis of a regression equation of the log K_{ow} and the effect concentrations for several aquatic organisms. This means that for substances with a similar non-specific mode of action, for which effect concentrations are lacking, effect concentrations can be predicted using these QSARs.

Estimated chronic toxicity data can be used as input in extrapolation models. QSARs for 19 aquatic species of different taxonomic groups are available (Van Leeuwen et al., 1992), from which NOECs can be estimated and used in deriving ERLs (Van de

Plassche and Bockting, 1993). The QSARs are provided in Annex 8. NOECs estimated with these QSARs subsequently serve as input for the method to derive ERLs, Section 6.2. The NOECs are used to calculate an HC5 under the assumption of a log-normal distribution according to Aldenberg and Jaworska (2000). QSAR-based HC5-values are presented in Appendix 8. If doubts arise on the validity of selected NOECs (in case only few data are available) for compounds with a non-specific mode of action, QSARs can be used for the purpose of comparison and choices will be made based on expert judgement.

3.3.3.2 Terrestrial toxicity data

For the terrestrial environment, toxicity data on terrestrial species are searched for, as well as effect data on microbiological processes and enzymatic activities. The data on microbial and enzymatic processes are commonly expressed as a NOEC or as an EC_x value (x=0-100%). These values are usually recalculated, cf. Section 4.4.1.

The results of terrestrial toxicity tests are separated for species and processes since processes are performed by many (micro) organisms that are not known and tested individually¹. Table 6 provides the information on relevant experimental conditions and results that are collected for terrestrial species. Basic data are collected and tabulated according to a specific format (Annex 3B) and reported (Annex 9).

Table 6. Information on relevant experimental conditions and results that are collected for toxicity studies on terrestrial species. The underlined parameters are required.

Conditions	Parameters
Organism	<ul style="list-style-type: none"> • <u>Species or process</u>, taxon, strain, scientific name, <u>age</u>, <u>weight</u>, <u>length</u> or <u>life stage</u>
Substance	<ul style="list-style-type: none"> • <u>Purity</u> (e.g. analytical grade or in percentage) • For metals and other naturally occurring substances: <u>added concentration corrected for background?</u> • Substance added in solution?
Soil	<ul style="list-style-type: none"> • Type of soil according to American soil type classification (Annex 4), and sample depth • <u>Soil characteristics</u> (organic matter content, clay content, pH, CEC)
Test conditions	<ul style="list-style-type: none"> • Is substance <u>analysed</u>? • Temperature • Soil to water ratio • <u>Duration</u> of the test (hours, days or months) • <u>Type of endpoint</u> (growth, shoot growth, reproduction, number of young, cocoon production, sperm production, etc.)
Results	<ul style="list-style-type: none"> • <u>Expression of endpoint</u> (EC_x, NOEC, etc.) • <u>Recalculation</u> of endpoint in standard soil • <u>Reference</u> of the study

¹ Statistical significance of the differences is tested according to section 4.4.1.2

3.3.3.2.1 *Terrestrial organisms, microbial processes and enzyme activity*

If at least 4 reliable NOEC values are available for both soil organisms of different taxonomic groups and 4 NOEC values for microbial processes and/or enzymatic activity, only a short overview of the acute toxicity data is required. When reliable chronic toxicity data are available for species from less than 4 taxonomic groups, an evaluation of acute toxicity literature is required.

3.3.3.2.2 *Insufficient data*

When insufficient data on terrestrial species are available the Equilibrium Partitioning method (EqP-method) is applied to derive ERLs for soil (Section 6.5). In the latter case, soil/water partition coefficients are required. MPCs for metals in soil or sediment can be derived from MPCs in water applying a modified equilibrium partitioning method (modified EqP-method, Section 6.5.1).

3.3.3.3 *Sediment toxicity data*

For sediment, in principle effect data on microbiological processes, enzymatic activities and benthic species are separated analogous to the separation for soil data. The data set is often too small (if available at all) to warrant separate treatment of processes and species, and separate data sets have so far not been used.

In most cases no sediment toxicity data are available at all. Therefore, for sediment, the Equilibrium Partitioning method (EqP-method) is usually applied to derive ERLs for sediment (Section 6.5). To apply the EqP-method, sediment/water partition coefficients are required (section 3.3.2). Hardly any ecotoxicological data are available for metals and metalloids, and MPCs and SRCs can be derived from ERLs in water applying a modified equilibrium partitioning method (modified EqP-method, section 6.5).

3.3.3.4 *Air toxicity data*

For air, toxicity data are collected on all organisms if available. Toxicity data for air have so far been collected for volatile compounds such as non-halogenated monocyclic aromatic hydrocarbons (e.g. benzene, styrene, toluene), halogenated monocyclic aromatic hydrocarbons (e.g. chlorobenzenes) and aliphatic chlorinated hydrocarbons. (Rademaker et al., 1993). The majority of toxicity data is mostly for mammals and occasionally for plants. It is proposed to use the same minimum data requirements for water (Table 5) and tabulate these (Annex 3A) for further reference. Annex 11 lists the data requirements for the calculation of an MPC for air, based on human toxicological information.

3.3.3.5 *Secondary poisoning*

Some contaminants may accumulate through the food chain and thus may have toxic effects on higher organisms, such as birds and mammals. If a substance is potentially bioaccumulative, as determined from the criteria in Table 7, additional data are required. For metals this is considered on a case-by-case basis.

One terrestrial food chain 'soil → earthworm → worm-eating predators' is considered. Ecotoxicological data for birds and mammals, and Bioaccumulation Factors (BAFs, earthworms-soil) for earthworms are searched for when secondary poisoning needs to be assessed, according to Table 8. Two aquatic food chains are considered to assess the potential for secondary poisoning: 'water → fish → fish-eating predators' and 'water → mussel → mussel-eating predators'. Ecotoxicological

data for birds and mammals, and BCFs or BSAFs for fish and mussels are collected, according to Table 8.

Table 7. Conditions for considering secondary poisoning

Characteristics	Conditions
Physico-chemical characteristics	<ul style="list-style-type: none"> Log K_{OW} > 3¹ and molecular weight < 700²
Biological characteristics	<ul style="list-style-type: none"> Low metabolisation and or excretion rate
(Organo)metals	<ul style="list-style-type: none"> Suspicion confirmed by consulted literature

Table 8. Data requirements for considering secondary poisoning

Requirements	Parameters
Bird and mammal toxicity	<ul style="list-style-type: none"> As in Table 2, <u>reporting the exposure route and exposure (e.g. diet concentrations)</u>
Bioconcentration/bioaccumulation factors	<ul style="list-style-type: none"> BCF, BAF or BSAF BCFs, BAF or BSAFs reported as or recalculated to whole body (fw). For mussels, BCFs/BSAFs for whole body are based on the soft tissue.

¹ In the context of admission of pesticides, a BCF for fish of > 1000 is considered to be a trigger for secondary poisoning. Given the fact that $BCF(wwt) = 0.05 * KOW$, with 0.05 = lipid volume, and a fish density of 1 kg/l, the $\log Kow = 4.3$.

² This cut-off value is mentioned in the TGD (ECB, 1996) but should be used with caution. Other factors are important as well: molecular size, (membrane) solubility and time to equilibrium (cf. Mayer, 2000; Verbruggen, 1999).

4. Data evaluation and treatment

This chapter starts with an overview of the main aspects of reliability of toxicity data, after which ecotoxicological endpoints, test conditions, data selection and the evaluation of secondary poisoning is discussed.

4.1 Reliability and usefulness of studies

The starting point in judging the reliability of all studies are the criteria established by the OECD (OECD, 1987). Tests for which no OECD guidelines are available, are judged case by case, with the criteria established by the OECD as a key source. Confidential reports and public literature have a different status for the regulatory authorities on pesticide registration, since public literature generally does not comply with the data requirements for pesticide registration. This is not seen as a problem for MPC derivation purposes.

For the evaluation of studies in the context of pesticide registration, a reliability index (RI) is used for the designation of the reliability of a study (Mensink et al., 1995). The studies, confidential reports and public literature, will be evaluated according to the criteria mentioned in this chapter. If the studies are judged useful and reliable (i.e. RI is 1 or 2) they will be used to derive ERLs in the context of pesticide registration (Table 9). Studies classified as unreliable (RI of 3) will still be indicated in the final report and designated as ‘not included in deriving ERLs’.

Table 9: Reliability Index for qualifying studies.

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

4.2 Fate and behaviour

For partition coefficients, data are selected or recalculated for further use in the extrapolation methods. The selection of data will result in a set of toxicity data, which is to be used for extrapolation and tabulated in the final report (Annex 3C, Annex 9).

4.2.1 Partition coefficients

For partition coefficients (K_p), only results from batch experiments are considered reliable (Bockting et al., 1992; Bockting et al., 1993). Also studies are considered reliable if performed according to the OECD-guidelines (OECD, 1984). Only studies in which the humus content, organic matter content or the organic carbon content is reported are accepted. In addition, well-performed field data may also be accepted.

For organic substances, the median log K_{oc} from all available experimental partition coefficients is calculated. This value is converted into the K_p value for a standard soil or sediment by multiplying it by 0.0588 (=organic carbon content of the standard soil):

$$K_{p(ssoil)} = K_{oc} * f_{oc} \quad (9)$$

in which:

$K_{p(ssoil)}$ = partition coefficient for standard soil or sediment [l/kg]
 K_{oc} = organic carbon-normalised partition coefficient [l/kg]
 f_{oc} = fraction organic carbon of standard soil (0.0588 [g oc/ g dw soil])

For metals, empirical distribution coefficients are searched for, e.g. for suspended matter/water, sediment/water and soil/water. The results are presented in specific tables (see Section 5.4).

4.3 Ecotoxicological data

4.3.1 Preferred endpoints

With respect to the ecotoxicity studies from the literature, only ecotoxicological endpoints are included that affect the species at the population level. In general these endpoints are survival, growth and reproduction. Reproductive effects include (histopathological) effects on reproductive organs, spermatogenesis, fertility, pregnancy rate, number of eggs produced, egg fertility, hatchability etc. (Slooff, 1992). For secondary poisoning, additional reproduction effects may be available: fertility, pregnancy rate, number of live fetuses, pup mortality, eggshell thinning, egg production, egg fertility, hatchability, and chick survival (Romijn *et al.*, 1993). For the terrestrial compartment, microbial processes and enzyme activities are also taken into account.

4.3.2 Other endpoints

Other ecotoxicological endpoints may be used for the goal of additional evidence for comparison with ERLs that are still derived from the preferred endpoints:

- The first criterion for acceptance depends on the ecological relevance of the endpoint, e.g. immobility in tests with daphnids.
- The second criterion is that a compound has a specific toxic mode of action. In that case, endpoints should be selected based on expert knowledge of the toxic mode of action. In the case of chemicals suspected of endocrine disruption such as

phthalates, in vitro and in vivo screening tests for (anti-) estrogenic/androgenic potency were evaluated as well (VanWezel et al., 2000b).

Such selected tests are used in two ways:

- To verify that ERLs, derived from the preferred endpoints are protective for specific toxic mode of actions.
- As supporting evidence in the evaluation of the preferred toxicity endpoints.

Expert judgement is needed to compare these findings with the ERLs based on the preferred endpoints, since specific (molecular or genetic) biomarkers are difficult to interpret in terms of population fitness or viability.

Thus far, no methodology is available to evaluate studies in which carcinogenicity or mutagenicity is taken as endpoint. In those cases it is still not clear whether species are affected at the population level.

4.3.3 Test conditions

For derivation of ERLs, background information such as physical/chemical properties and properties concerning degradation/metabolite formation is needed. Environmental fate and behaviour of compounds might influence the outcome of standard laboratory test and thus influences the ERLs. In general, studies need to be conducted according to international accepted guidelines, such as the OECD guidelines (OECD, 1987). If study designs deviate from those guidelines, they may still be accepted as relevant studies. The following quality criteria are taken into account in evaluating the studies:

- The purity of a test substance. The purity of the tested substance has to be at least 80%. For pesticides with a purity of 80-95% data on the composition of the pesticide and its impurities can mostly be found in additional information. Studies with substances with a purity between >20 and <80% are included in the table 'Toxicity data from deviating tests' because these are not used for extrapolation but can still be very informative. Granulates and substances with a purity <20% are not included in the tables. An exception is made for granulates and wettable powders, where purity between 20 and 80% is acceptable if the absence of toxicity of the carrier compound is established or made plausible.
- Toxicity data of metal compounds are always expressed in quantities relating to the element and not as the salt.
- Studies using animals from polluted sites are rejected.
- In aquatic studies, concentrations that exceed 10 times the aqueous solubility are rejected.
- A maximum of 1 mL/L of solvent used for application of the test substance in aquatic studies is accepted, deviating from OECD test guidelines¹.
- Solvent use in terrestrial studies may not exceed a value of 100 mg/kg if the solvent was not allowed to evaporate from the soil before the test animals were introduced. This is adapted from the concept guidelines for studies on Folsomia. If the animals were introduced after evaporation of the solvent, the initial solvent use is allowed to reach a value of 1000 mg/kg, under the condition of no negative

¹ If more than 0.1 ml/l solvent is applied the amount of solvent is mentioned in a footnote to the aquatic toxicity table. When the amount of solvent is not reported this is mentioned in a footnote.

effects¹, the use of a solvent can cause negative or positive effects (e.g. because of higher availability of nutrients). In case of positive effects the test will not be used for evaluation.

- The recovery of the substance in aquatic studies needs to be 80% or more.

4.3.4 Test duration

The decision on whether a toxicity test is acute or chronic depends on the species that is tested and its life cycle. In view of the life span of the species, acute toxicity will always represent a relative short period of time. The exact length of the time period depends on the physiological nature of the species in question and its life cycle.

Chronic toxicity represents a complete or partial life cycle including sensitive young stages or one or more reproduction cycles, the exact length of the time period again depending on the physiological nature and life cycle of the species.

For a number of species from several taxonomic groups the OECD has set up a number of standard fixed test durations. The length of these standard test durations can be found in the OECD guidelines for testing of chemicals. The test endpoints are commonly expressed as an acute LC50 or EC50 for short-term tests with a duration of less than four days, or as a chronic NOEC for long-term tests with a duration of four or more days. For microorganisms and algae, NOECs may be derived from experiments lasting less than four days.

In addition to these guidelines the following distinctions are drawn for the purpose of deriving ERLs:

- a) Algae, Bacteriophyta, Protozoa: a test duration of maximal 4 days; NOEC data over a test period of 3-4 days are defined as chronic. Tests, in which longer exposure durations are used, will only be taken into account if the control population is still in the exponential growth phase. EC50 data from such tests can be recalculated conform Section 4.4.1.
- b) Crustacea and Insecta: test durations of 48 or 96 hours are considered to be acute.
- c) Pisces, Mollusca and Amphibia: for these species 96 hours is the time span of the standard acute toxicity test. Early life stage tests (OECD 210) egg and sac-fry stage tests and 28 day growth tests (both subject of discussion at OECD) are considered chronic tests. The prolonged toxicity test (OECD 204) is considered an acute test.
- d) Tests with deviating test durations (chronic and acute), are placed in the table 'toxicity data from deviating tests' (e.g. 48 h, fishtest; 14 d, LC50, fish test).

¹ If the added solvent is between 100 and 1000 mg/kg, the amount of solvent is mentioned in a footnote to the soil toxicity data table.

4.4 Data selection and treatment

Toxicity data, data are selected or recalculated for further use in the extrapolation methods. The selection of data will result in a set of toxicity data, which is to be used for extrapolation and tabulated in the final report (Annex 9).

4.4.1 Aquatic toxicity data and general remarks

4.4.1.1 General calculations (all compartments)

Toxicity data are selected in order to obtain one single reliable toxicity value for each compound and species. This refers to data for a single type of endpoint, e.g. NOEC or LC50. One value per species is required as input in the subsequent extrapolation method (Chapter 6). It is possible and often necessary to use both acute and chronic data in deriving ERLs (cf. Chapter 6). Therefore, acute and chronic toxicity data are weighed over the species as follows (Slooff, 1992):

- If for one species several toxicity data, based on the same toxicological endpoint, are available, the geometric mean value is calculated.
- If for one species several toxicity data, based on different toxicological endpoints are available, the lowest value is selected. The lowest value is determined on the basis of the geometric mean, if more than one value for the same parameter is available.
- In some cases data for effects on different life-stages are available. The most sensitive result will be used in the extrapolation, e.g. one most sensitive life-stage, else the first rule applies.

The following procedure is used to convert available toxicity data into No-Observed Effect Concentrations (NOECs):

- The highest reported concentration, not statistically different from the control at $p < 0.05$, is regarded as the NOEC if it is not the highest tested concentration;
- The highest concentration showing 10% effect or less is considered to be the NOEC if no statistical evaluation is possible;
- If only a Lowest-Observed Effect Concentration (LOEC) is reported, the LOEC is converted into a NOEC as follows (ECB, 1996; section 3.3):
 - $10 < \text{LOEC} < 20\%$ effect: $\text{NOEC} = \text{LOEC}/2$. If at least two values are available, see footnote ¹.
 - $\text{LOEC} \geq 20\%$ effect and a distinct concentration-effect relationship is available: $\text{NOEC} = \text{EC}_{10}$ ¹
 - $\text{LOEC} \geq 20\%$ effect and no distinct concentration-effect relationship is available²:
 - $20 \leq \text{LOEC} < 50\%$ effect: $\text{NOEC} = \text{LOEC}/3$;
 - $50 \leq \text{LOEC} \leq 80\%$ effect: $\text{NOEC} = \text{LOEC}/10$;
 - If other test results are available within the same taxonomic group with distinct concentration-effects relationships, these are used to verify the above

¹ A log-logistic dose-response curve can be fitted with the EXCEL solver using non-linear regression, cf. Van Beelen et al., 1991. At least two data points are needed, preferably both $< \text{EC}_{70}$.

² In the draft EU-RAR on Zinc (RIVM/TNO, 1999), different limits are used: 10 to 30% ($\text{LOEC}/3$) and 30-50% ($\text{LOEC}/10$) is used, which are more reasonable in view of the often used factor of 10 between the $\text{L(E)}\text{C}_{50}$ and the NOEC and are therefore advised in future.

mentioned factors. If for instance a reliable acute-chronic ratio is available within the same taxonomic group this ratio is used instead of one of the factors mentioned above. 'Reliable' is based on expert judgement.

- If the highest tested concentration is not statistically different from the control, NOECs are reported as $\text{NOEC} \geq [\text{highest observed no-effect concentration}]$. These may only be used for toxicity evaluation if they are the only available studies. In that case, the highest observed no-effect concentrations do not adequately describe the variation in response between organisms. For that reason, statistical extrapolation is not advised and safety factors should be used (preliminary risk assessment, Section 6.2).
- The 'Toxische Grenzkonzentration' (TGK) or 'Toxic Threshold' (Bringmann and Kühn, 1977) is regarded as a NOEC;
- If a 'Maximum Acceptable Toxicant Concentration' (MATC) is presented as a range of two values, the lowest is selected as NOEC; if a MATC is presented as one value, the $\text{NOEC} = \text{MATC}/2$.
- When effective concentrations were only approximately established, the \leq or \geq values are reported in a separate table 'Toxicity data from deviating tests'. Data for water are expressed as dissolved concentrations, while often total concentrations are measured or reported. Dissolved concentrations can be calculated from total concentrations using the following equation:

$$C_{\text{dissolved}} = \frac{C_{\text{total}}}{1 + Kp_{\text{pm}} \cdot [\text{pm}]} \quad (10)$$

with:

$C_{\text{dissolved}}$	= dissolved concentration in water [mg/l]
C_{total}	= total concentration in water (in [mg/l])
Kp_{pm}	= particulate matter/water partition coefficient [l/kg]
$[\text{pm}]$	= concentration of particulate matter in water [kg/kg]

For reporting ERLs for water (cf. section 5.6), recalculation of ERLs for the dissolved phase to the total water phase (i.e. dissolved and suspended) is required (Annex 10).

4.4.1.2 Statistical analysis

When distinct differences seem to exist between two groups, e.g. between fresh- and saltwater organisms, or between target and non-target species, statistical analysis must be performed. If no prior knowledge exists which group is more sensitive than the other, an unpaired t-test with a two-tailed P value should be chosen. The unpaired t test compares two groups, based on the assumption that the two populations are Gaussian. If the variance of the two groups is not equal, Welch's modified t-test can be employed (available in most statistical software). If it is known beforehand which group is more sensitive (in case of target species), a one-tail P value must be chosen. If the prediction (of the most sensitive group) was wrong, the P value reported by the statistics program should be ignored; it should be stated that $P > 0.50$. The assumption of a Gaussian distribution is tested using the Kolmogorov-Smirnov test where the mean and SD are estimated from the sample of NOEC data (e.g. with GraphPad Prism, 1996).

4.4.2 Soil toxicity data

For soil, toxicity data on terrestrial species as well as on microbial and enzymatic processes may be available. Due to the nature of the endpoint, the latter data describe the performance of a process 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 cannot be averaged with single species tests, because of the fundamental differences between them (Van Beelen and Doelman, 1996)¹.

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, one geometric mean value is selected. In specific cases, isolated microorganisms or fungi are used in microtests and are regarded as individual species and added to the set of species NOECs.

The route of exposure used in a soil toxicity experiment has to be in agreement with the natural route of exposure of the species considered. If this is not the case, the study will not be used for derivation of the ERLs². The following criteria are used:

- species which live in the soil have to be exposed through soil (e.g. *Folsomia candida*);
- species which live on the soil, in the litter layer, have to be exposed through the food (e.g. *Orchesella cincta*). Food exposure must be recalculated to soil concentrations using normalisation equations (cf. Section 4.4.2.1).

4.4.2.1 Recalculation to standard soil

Because many different soils are used in terrestrial toxicity tests, normalisation of the terrestrial test results takes place (Denneman and Van Gestel, 1990). All data on the sensitivity of species are recalculated for a standard soil, i.e. a soil that contains 10% organic matter (H) and 25% of clay (L).

The following equation is used for normalisation of studies with metals:

$$ECx_{(soil)} = ECx_{(exp)} \frac{R_{(soil)}}{R_{(exp)}} \quad (11)$$

in which:

$ECx_{(soil)}$ = Effect Concentration; normalised NOEC or LC50 for standard soil (or sediment) in mg/kg dw

$ECx_{(exp)}$ = Effect Concentration; NOEC or LC50 for soil (or sediment) as used in the experiment in mg/kg dw

¹ It is proposed that the data for species and processes are analysed for statistical significant differences and may be combined if no significance is established. The significance is based on a two-sided T-test (without assumptions on the most sensitive group) with a significance level $\alpha = 0.05$.

² Deviating studies will be documented in a separate table

- $R_{(soil)}$ = Reference-value for standard soil or sediment (H=10%, L=25) in mg/kg dw
- $R_{(exp)}$ = Reference-value for soil or sediment used in the experiment (H=y%, L=z%) in mg/kg dw.

The Reference values for metals in soil are based on so-called reference-lines (Table 10). These reference lines were derived from a regression analysis on 90th percentiles of ambient background concentrations from various, relatively unpolluted sites in The Netherlands with percentage clay and organic matter content of these soils (Edelman, 1984; De Bruijn and Denneman, 1992).

Table 10. Empirical reference lines for calculating the background concentration for different Dutch soils and sediments (De Bruijn and Denneman, 1992). H = percentage of organic matter in soil or sediment (based on dry weight), L = percentage of clay content in soil or sediment (based on dry weight). Cb = the background concentration for standard soil or sediment (in mg/kg dry weight), where H = 10%, and L = 25%.

Metal or Metalloid	Reference line for Soil or Sediment	Cb
Antimony (Sb)	3.0	3.0
Arsenic (As)	15 + 0.4 (L + H)	29
Barium (Ba)	30 + 5L	155
Beryllium (Be)	0.3 + 0.033L	1.1
Cadmium (Cd)	0.4 + 0.007(L + 3H)	0.8
Chromium (Cr)	50 + 2L	100
Cobalt (Co)	2 + 0.28L	9.0
Copper (Cu)	15 + 0.6(L + H)	36
Lead (Pb)	50 + L + H	85
Mercury (Hg)	0.2 + 0.0017(2L + H)	0.3
Molybdenum (Mo)	0.5	0.5
Nickel (Ni)	10 + L	35
Selenium (Se)	0.7	0.7
Thallium (Tl)	-	1.0
Tin (Sn)	4 + 0.6L	19
Vanadium (V)	12 + 1.2L	42
Zinc (Zn)	50 + 1.5(2L + H)	140

For organic substances, the literature results are normalised on organic matter content:

$$ECx_{(soil)} = ECx_{(exp)} \frac{H_{(soil)}}{H_{(exp)}} \quad (12)$$

in which:

$ECx_{(soil)}$ = Effect Concentration: normalised NOEC or LC50 for standard soil (or sediment) in mg/kg dw

$ECx_{(exp)}$ = Effect Concentration: NOEC or LC50 for soil (or sediment) as used in the experiment in mg/kg dw

$H_{(soil)}$ = Organic matter content of standard soil (or sediment) (H= 5 or 10%) in mg/kg

$H_{(exp)} =$ Organic matter content of soil or sediment used in the experiment ($H = y$ %) in mg/kg dw.

The standard soil is 10% organic matter for deriving ERLs, the organic carbon content of the standard soil is 5.88%. The standard soil in the context of plant protection products is 4.7% organic matter. The type of standard soil should be mentioned in the tables where ERLs for standard soil are presented.

ERLs for specific soils are recalculated taking organic matter and clay content into account. Two cases can be distinguished: calculation for specific soils from a standardised ERL or recalculation of toxicity data to a standardised soil. For such transformations, specific limitations apply. For soils with a low organic matter content, i.e. $H < 2\%$, H is set at 2%. Similarly, for soils with a high organic matter content, i.e. $H > 30\%$, H is set at 30%. However, for PAHs, for soil with an organic matter content of less than 10% or more than 30%, the percentage of organic matter is set at 10 and 30%, respectively. If animals are fed contaminated organic food, the food is considered to be organic matter in the soil. The same normalisation rules apply for food as listed above for recalculation to soil.

4.4.3 Sediment toxicity data

Sediment toxicity data are recalculated for standard sediment, i.e. sediment that contains 10% organic matter (H) and 25% of clay (L). The same equations as for soil are used (section 4.4.2.1) for the normalisation of sediment toxicity studies with metals (Equation 1) and organic substances (Equation 2). For transformations or standardisation to soils, specific cut-offs for organic matter apply as mentioned above for soil.

Protocols for toxicity studies carried out in sediment-water systems are still in development (Burton, 1992; Ciarelli et al. 1995, 2000). The evaluation of these studies is performed but is not supported by international accepted guidelines.

However, the following points should be considered:

- Sediment characteristics such as % organic carbon, particle size distribution, field or standard sediment,
- Amounts of sediment and water,
- Test method: static or flow-through, with flow-rate,
- How was the toxicant added to the test system,
- Analysis of the toxicant concentration in sediment and/or in water,
- Are sediment and water suspended or is the sediment settled down on the bottom of the test vessel,
- Are the toxicant concentrations in sediment and water in equilibrium,
- What is the exposure route of the test organisms,

The results are presented in tables, analogous to those for aquatic toxicity (cf. Chapter 5.1).

4.4.4 Air toxicity data

For plants, birds and insects, no international accepted guidelines exist for exposure via air although plant testing has received much attention during the past few years. In addition to the general guidelines of Chapter 4, expert judgement may be needed

using OECD guidelines for assessing study design. The evaluation of air toxicity data to derive an MPC for humans is described in Annex 11.

For volatile substances, the majority of studies is conducted with rodents for which OECD guidelines are present (cf. section 4.4.6.3). Recalculation of toxicity data may be needed. In air exposure experiments, both L(E)C50s and NOEC values are corrected for continuous exposure (24h/d, 7d/w):

$$NOEC \text{ _or_ } L(E)C50 = NOEC \text{ _or_ } L(E)C50(\text{exp}) \cdot \frac{D}{7} \cdot \frac{H}{24} \quad (13)$$

with :

D = number of exposure days per week

H = number of exposure hours per day (Rademaker et al, 1993).

4.4.5 Field studies

4.4.5.1 Aquatic field studies

Results from (semi-)field studies such as microcosm, mesocosm, macrocosm studies, enclosures, experimental streams or true field studies are sometimes available (Van Leeuwen *et al.*, 1994). Such studies are used for comparison with ERLs derived using single-species toxicity data (Chapter 6) and are part of the Preliminary Risk Analysis part of a standard report (Annex 9). These (semi-field) studies are used for verification of ERLs as derived according to Chapter 6, but usually not as input for derivation of ERLs. At present, a set of guidelines from the HARAP workshop is available (Campbell et al., 1998) and work is in progress to implement it for deriving ERLs. In general these studies are difficult to interpret. A set of criteria developed by Emans et al. (1993) can serve as a temporary tool for evaluation:

- A distinct concentration-effect relationship should be obtained;
- A reliable MS (multiple species) NOEC should be derived;
- Several taxonomic groups, in more or less natural ecosystems, should be exposed to one test concentration for a longer period;
- In each experiment several concentrations should be tested, consisting of one control and at least two test concentrations;
- Each test concentration should have at least two replicates;
- The concentration of the test compound should be measured several times during the experiment;
- Physico-chemical parameters like pH, temperature and hardness should be measured;
- Apart from effect parameters like population density and biomass also effect parameters at higher integration levels such as species diversity and species richness should be measured.

4.4.5.2 Terrestrial field studies

Protocols for soil toxicity studies carried out under field conditions are not existing. For evaluation of these studies the following points of attention can be given:

- Soil characteristics (especially % OM and % clay in view of conversion to standard soil);
- Application method (pressure injected, spraying, incorporation in soil or mixed);
- Number of applications and time intervals;

- Number of plots and number of replicates;
- Plot size and size of untreated strips;
- Randomization of plots;
- Information on the control used;
- Sample size and number of samples per plot;
- Sample time;
- Sample method/technique (electricity, surface 10 cm etc.);
- Crop planted on soil;
- Statistical analysis method.

The results are presented in tables (see Chapter 5.1).

4.4.6 Secondary poisoning

Some contaminants may accumulate through the food chain and may thus exert toxic effects on higher organisms, such as birds and mammals. If the substance is potentially bioaccumulative, as determined from the criteria in Table 7 (Section 3.3.3), toxicological data on the sensitivity of birds and mammals and BCFs for worm, fish and mussel must be searched for. For metals this is considered on a case-by-case basis. Toxicity data for birds and mammals and BCFs, BAFs or BSAFs are tabulated (Section 5, Annex 3D) and documented in the final report (Annex 9).

4.4.6.1 Bioconcentration factors

The BCF can be measured or calculated. The steady-state BCF is the ratio between the concentration in the organism and the concentration in a steady state (or equilibrium) situation. When uptake and depuration kinetics are measured, the kinetic BCF can be calculated from the quotient of the uptake and depuration rate constants:

$$BCF = C_{organisms} / C_{water} \text{ or } k_1 / k_2 \quad (13)$$

With $C_{organism}$ = concentration in organism [g.g⁻¹]
 C_{water} = concentration in water [g.l⁻¹]
 k_1 = uptake rate constant [g.g⁻¹.d⁻¹]
 k_2 = depuration rate constant [g.g⁻¹.d⁻¹]

Special criteria are available for bioconcentration factors (BCFs), bioaccumulation factors (BAF) or biota-to-sediment accumulation factors (BSAFs) derived from accumulation studies:

- A geometric mean is calculated from the available BCF values. If more than one value is available on a single species a geometric mean is calculated first, before an overall geometric mean (across species) is calculated.
- To establish if BCFs, BAFs or BSAFs are derived for steady state conditions, experimental duration must be taken into account. The experimental duration has to be sufficiently long in order to establish or approach a steady state between concentrations in water and the test species. In many studies it is often not clear whether steady state is reached. Therefore, an estimate is made of the duration of the uptake phase to reach 80% of the steady state (T80) based on the log K_{ow} according to OECD guidelines (1996). Only studies with an exposure time longer than the estimated T80 are included.

- If k_1 and k_2 are estimated from a (similar) reliable dynamic accumulation experiment, a steady state BCF/BAF/BSAF can be calculated, by using eqn. 13 (see e.g. guideline 305, OECD 1996). Parameter estimation of k_1 and k_2 (and thus BCF) is best performed at a time $\geq T_{80}$.
- No signs of overt toxicity should be observed. According to the OECD guidelines the highest exposure concentration should be less than 0.1 of the incipient LC50 for the test species and at least 10 times higher than the detection limit in water. Based on an evaluation of the literature for several compounds Van de Plassche (1994) concluded that these criteria are too stringent. Therefore deviating from OECD guidelines tests are evaluated in the following way: if mortality occurs the test concentration is excluded, while if nothing is reported on mortality by the author(s) all test concentrations higher than 0.20 times the 96 h LC50 of the test species are excluded.
- Experimental BCFs for fish and mussel are calculated as whole body concentration (wwt) divided by the concentration in water. Experimental BAFs for worms are calculated as concentration in worm (wwt) divided by the concentration in soil (dwt).
- If concentrations in soil are expressed as wet weight, a conversion factor of 1.25 [kg wwt/kg dwt] is used to convert concentrations in soil expressed as mg/kg wet weight to mg/kg dry weight, based on 20% humidity of wet soil.
- BCFs and BSAFs can be expressed on a wet weight basis if toxicity data are also given on the basis of moist food. If no information on the wet to dry weight ratio of organisms is available, the following dry to wet weight ratio's [kg dwt/ kg wwt] are used: bivalves 12 %, crustaceans: 9%; lean fish (e.g. roach) 25%, fat fish (e.g. eel) 38% (Hendriks et al., 1995) and earthworms 16% (Jager 1998).
- For metal BAFs and BSAFs can be normalised to a standard soil if regression analysis indicates a clear relation (i.e. $R^2 > 0.6$) between soil parameters and the BSAF and BAF. If such a relation is not observed, geometric mean BAFs and BSAFs are used.
- For organic substances, BCFs, BAFs or BSAFs are usually normalised to lipid content of the organism and in case of BAFs and BSAFs, to organic carbon content of the soil or sediment. This yields units for the BCF as [l/kg lipid], and [kg oc/kg lipid] for BAF and BSAF (cf. eqn. 14)
- NOECs for water exposure can be converted in equivalent NOECs expressed in organic carbon fractions of the sediment by using:

$$NOEC_{oc} = NOEC_w \cdot \frac{BCF_L}{BSAF_{LOC}} \quad (14)$$

with BCF_L = lipid normalised BCF [l/kg lipid]

$BSAF_{LOC}$ = lipid and organic carbon normalised BSAF [kg oc/kg lipid]

When experimental data are lacking, regression equations can be used to estimate the BCF for non-reactive lipophilic organic chemicals:

$$BCF\text{-fish}^1 \text{ [L/kg wwt]}: \quad BCF = 0.048 * K_{ow} \text{ (Mackay, 1982)}. \quad (15)$$

$$BCF\text{-mussel [L/kg wwt]}: \quad BCF = 0.013 * K_{ow} \text{ (Everts et al., 1992)}. \quad (16)$$

¹ For substances with a log Kow higher than 6, this equation should not be used. The TGD (ECB, 1996) suggests to use an empirical parabolic equation for these substances, but this equation is empirical and should be used with caution. Alternatives are discussed in Jager and Hamers (1997).

BCF-earthworm¹ [L/kg ww]: $BCF = 0.84 + 0.012 \cdot K_{ow}$ (Jager 1998). (17)
 To convert BCFs (such as eqn. 13) to a bioaccumulation factor related to soil or sediment, recalculation is performed according to:

$$B(S)AF \text{ [kg dw soil or sediment/ww]} = BCF / (f_{oc} \cdot K_{oc}). \quad (18)$$

Two options are available to calculate a BCF for earthworms, based on Jager (1998):

- 1) Use the theoretical model² (as if the toxicant in the worm is in equilibrium with that in pore water).
- 2) Use empirical relations as established from measured concentrations. Earthworm concentrations appear to be lower than predicted by the theoretical model. This may be due to absence of equilibrium, desorption limited uptake, experimental error etc. Given the fact that these conditions may vary over locations and time, the theoretical model is preferred. However, the empirical relations (presented as linear regression equations) may be used for comparison:

$$\log BCF = 0.87 \cdot \log K_{ow} - 2.00; \quad (19)$$

for non-ionic toxicants² and chlorophenols;

$$\log BCF = 0.94 \cdot \log K_{ow} - 2.43; \quad (20)$$

for non-ionic toxicants; excluding chlorophenols

4.4.6.2 Biota to Sediment Accumulation Factors

To evaluate secondary poisoning data, all data must be compared for a common exposure medium, i.e. water, soil or sediment. BSAFs derived from field data are preferred, to avoid lab-to field extrapolation problems. If water concentrations are needed, available BSAFs can be converted. In some cases, BSAFs based on concentrations in suspended matter (as applied in Smit et al., 2000) are reported instead of BCFs. If no monitoring data on corresponding dissolved concentrations in water are available, BSAFs are converted to BCFs using the equilibrium partitioning method, either by first calculating concentrations in the water and using this value to calculate the BCF:

$$C_{water} = \frac{C_{susp}}{K_{p,susp}} \quad (21)$$

and

$$BCF = \frac{C_{organism}}{C_{water}} \quad (22)$$

or, if concentrations in the organisms are not available, by directly converting BSAFs into BCFs:

$$BCF = BSAF \times K_{p,susp} \quad (23)$$

In some cases, BSAFs are preferred. This may be the case when compounds are very hydrophobic, are mostly associated with organic matter and concentrations in the

¹ The theoretical model is $BCF = \text{fractionWater} + \text{fractionFat} \cdot K_{ow}$ (Jager, 1998).

² Substances in the regression are chlorobenzenes, PCBs, PAHs, Dieldrin, DDT, Lindane, TCDD, a herbicide and some fungicides (Jager, 1998).

water are very low. In such cases, more emphasis is placed on sediment ERLs than ERLs for the (dissolved) water phase. In that case, BSAFs based on lipid-organic carbon partitioning can be used directly. For very hydrophobic compounds such as polychlorinated biphenyls (PCBs), it may be needed to recalculate NOECs or LC50s to values normalised on organic carbon content of sediments using BSAFs. Since these calculations are very specific, guidance on this issue is provided in Van Wezel et al. (2000a).

4.4.6.3 Toxicity studies with birds and mammals

Toxicity studies with birds and mammals are evaluated in order to assess possible effects due to secondary poisoning. This concerns subacute and (semi)chronic studies with mammals and acute and (semi)chronic studies for birds, all exposed via food. LC50 values for birds and NOEC values are derived. Relevant OECD guidelines are 205, 206, 407/409, 414/416, 451/453. Examples of standardised toxicity tables for birds and mammals are given in Annex 3E and detailed in Section 5.3.

Special reliability criteria are available for birds and mammals:

- Especially in acute dietary studies with birds repellency may occur, i.e. the animal is not inclined to eat due to the toxicant. In such a case, the outcome of the LC50 test is not only a reflection of the intrinsic toxicity of the tested chemical but also of decreasing food consumption leading to starvation. Therefore special attention is paid to, if available: food consumption pattern, the shape of the dose-mortality curve in time and the No Repellent Concentration. More guidance can be found in Luttik (1993).
- Endpoints for birds and mammals are described in Section 4.3. Especially in (semi)chronic studies with mammals, other less preferential endpoints are considered as well and often no NOEC is derived for mortality, growth or reproduction. Therefore, NOECs for other endpoints may have to be extracted from the original literature source. Reproduction studies are considered as chronic studies. Eggshell thinning is taken into account only if the effect is more than 20%.
- From chronic tests with mammals mortality is generally not a good endpoint. NOEC values can often not be derived because more than 20% mortality is reached in many tests in the second year, which cannot be ascribed directly to the test substance.
- If NOECs are reported as dose per kg body weight per day ($\text{mg} \cdot \text{kg} \text{ bw}^{-1} \cdot \text{d}^{-1}$), these values are converted to mg/kg food using conversion factors (Table 11) based on the inverse of the daily food intake (Romijn et al., 1991a,b, ECB1996). If specific data on daily food intake are available, the conversion values of Table 11 are corrected using this value. Caution must be taken if no steady-state is reached. In such cases, kinetic data should be taken into account to estimate whether steady state was reached.
- If BAFs or BSAFs are not in steady state, (as is often the case in feeding studies (expressed as $\text{mg}/(\text{kg} \text{ bw} \cdot \text{d})$) with hydrophobic chemicals), steady-state BAFs or BSAFs can be calculated. Then, k_1 and k_2 should be estimated from a (similar) reliable dynamic accumulation experiment and a steady state BCF/BAF/BSAF can be calculated by using eqn. 13 (see guideline 305, OECD, 1996). Parameter estimation of k_1 and k_2 (and thus BAF/BSAF) is best performed at a time $\geq T_{80}$. Parameter estimates should preferably be obtained from the species under consideration, since transfer across species neglects differences such as weight or

other allometric considerations that influence rate constants (Sijm and Van der Linde, 1995; Hendriks, 1995a,b).

Table 11: Conversion factors [kg bw.d/kg food] for recalculation of body weight concentrations to concentrations in food; birds and mammals.

Species	Conversion factor
Canis domesticus (dog)	40
Macaca spec. (rhesus monkey)	20
Microtus spec. (hamster)	8.3
Mus musculus (mouse)	8.3
Oryctolagus cuniculus (rabbit)	33.3
Rattus norvegicus > 6 weeks old (rat)	20
Rattus norvegicus < 6 weeks old (rat)	10
Gallus domesticus (chicken)	2
Mustela vison (mink)	10

4.4.6.4 Conversion of bird and mammal NOECs

All toxicity data, including those for secondary poisoning, are used as input for methods to derive ERLs following the advice of the Technical Soil Protection Committee (TCB, 1994; Kalf et al., 1999). In order to do so, all toxicity data should be expressed as exposure concentrations in a common environmental compartment, either soil or water. Conversion of all toxicity data to the organic carbon fraction of soil or sediment was employed in the case of Polychlorinated Biphenyls (van Wezel et al., 2000a, c.f. Annex 7). Pending the advice of the Dutch Health Council and the Technical Committee for Soil Protection, this method can not yet be recommended. It is advised to use this method as addition to the current one, and in a preliminary fashion for highly bioaccumulative substances (such as PCBs, dioxins, furans etc.) where the uncertainty in sorption coefficients and B(S)AFs is substantial. Data requirements are large and this may limit the use of this method.

All individual NOECs for birds and mammals are divided by either a BCF, BAF or BSAF to obtain concentrations in water or soil. Together with the L(E)C50 or NOEC values for aquatic or soil organisms, these values are used as input data for the preliminary method or the statistical extrapolation method as shown in Figure 3. All toxicity data are combined¹ since the conceptual idea for deriving ERLs is the protection of all species in the ecosystem.

The following steps are employed to assess toxicity data for birds and mammals:

1. NOECs for birds and mammals, all (recalculated to) concentrations in mg/kg food, are converted to mg/l water or mg/kg soil by dividing the NOEC by the BCF or BSAF and multiplying by a correction factor for caloric content²:

¹ ERLs based on secondary poisoning reported before the year 2000 were based on separate data sets for secondary poisoning and direct toxicity.

² Based on differences in the caloric content of food provided to caged animals and that of their natural food, conversion factors have been discussed by several authors (Dutch Health Council (1993), Romijn et al., 1993; Traas et al., 1996). Ruys and Pijnenburg (1991) derived the conversion factors for fish and mussels, based on a large review. The conversion factor for earthworms is based on Westerterp et al. (1982).

$$NOEC_{water, fish-to-predator} = \frac{NOEC_{predator}}{BCF_{fish}} \times 0.32 \quad (24)$$

$$NOEC_{water, mussel-to-predator} = \frac{NOEC_{predator}}{BCF_{fish}} \times 0.20 \quad (25)$$

$$NOEC_{soil, worm-to-predator} = \frac{NOEC_{predator}}{BCF_{worm}} \times 0.23 \quad (26)$$

2. If more than one NOEC is available for the same parameter, the geometric mean of the NOECs for that species is calculated (cf. 4.4.1).
3. For the aquatic compartment, the lowest of the two NOEC values (via fish or via mussel BCFs) per test species is selected. The lowest NOECs for all bird and mammal species are combined with the other direct toxicity data on aquatic species as input for the methods of Chapter 6. For the terrestrial compartment, the NOECs for worm eating birds or mammals are combined with other direct toxicity data on terrestrial species as input for the methods of Chapter 6.
4. The combined data set is used for derivation of the ERL (Fig. 3, after Smit et al., 2000). To gain insight in the relative sensitivity of vertebrates as compared to that of other species, the MPC based on secondary poisoning alone is calculated as well, reported and compared to that of the direct toxicity data set (separate sets, Fig. 3). MPCs based only on data for birds and mammals are estimated from the converted NOECs for birds and mammals using equations 24 to 26.

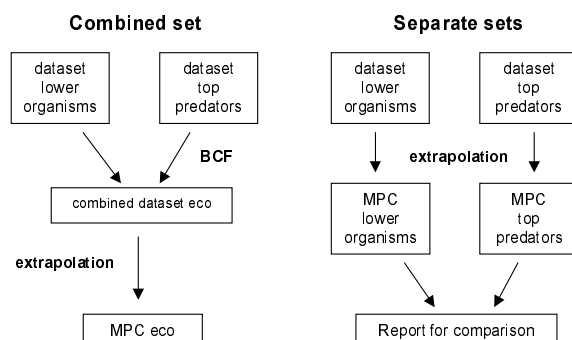


Figure 3: Secondary poisoning as included in the derivation of MPCs. In the combined set method, the data are combined. For the purpose of comparison, MPCs for lower organisms and top predators are reported separately (after Smit et al., 2000).

5. Data tables

The toxicity data, data on sorption coefficients, and bioconcentration factors (or BAFs or BSAFs) needed for calculation of secondary poisoning, are evaluated according to the procedure described in Chapter 4. This results in a set of data that are to be used in deriving the environmental risk limits and data from deviating tests that may help interpreting the data set as a whole. This chapter describes the format that is used at RIVM for tabulating the data and documenting specific aspects of the underlying studies. Furthermore, specific details about documenting studies and recalculations are mentioned for several evaluation criteria. Example tables are shown in Annex 3A-3E.

5.1 Aquatic toxicity data

Examples of standardised aquatic toxicity tables are given in Annex 3A. The column entries in the toxicity tables are discussed below. Aquatic toxicity data are subdivided and tabulated as

- chronic toxicity freshwater organisms
- chronic toxicity marine organisms
- acute toxicity freshwater organisms
- acute toxicity marine organisms
- toxicity data from deviating tests

This format is also used for air toxicity data if available. Sections 5.1.6 to 5.1.8 are not relevant for air toxicity data. In case of air data, volume is indicated in cubic meters (m³).

5.1.1 Species

The species name should be mentioned in the table, and listed under the correct taxonomic group (Annex 3A). The main taxons used are shown in Table 12.

Table 12: Taxonomic classification of aquatic organisms

Bacteria	Rotatoria
Cyanophyta	Nematoda
Protozoa	Mollusca
Algae (e.g. Chrysophyta, Chlorophyta)	Annelida
Macrophyta	Crustacea
Fungi	Insecta
Coelenterata	Pisces
Echinodermata	Amphibia
Platyhelminthes	

5.1.2 Species properties

Age, size, weight or lifestage is mentioned, following the name of the organism. The toxicity data of animals with different age, size or weight are presented individually in the tables.

When the tested organisms are collected from field populations, this fact is mentioned in a footnote with the duration of the acclimation period. When the authors report that the organisms are originating from a contaminated area the test is not included.

5.1.3 Analysis of test compound

If the concentration of the test compound is measured during the test, and results are expressed as measured values, **Y** is placed in this column. If not measured during the test or not mentioned, **N** is placed in column.

If in static or renewal tests, samples are analysed at different points of time, the geometric mean of the measured values is reported. When the initial concentration is not measured and one or more samples during the test are, the geometric mean of the initial nominal and the measured concentration(s) is reported. In continuous flow experiments the concentrations are usually reported as mean measured values, no further calculations are necessary.

5.1.4 Test type

The following test types are distinguished:

- R renewal system (semi-static)
- S static system
- CF continuous flow system
- IF intermittent flow

5.1.5 Substance purity/compound

This column can be either 'substance purity' (for non-metal compounds) or 'test compound', if the tested compounds are metal salts.

5.1.5.1 Substance purity

The purity of the tested substance has to be at least 80%. Exceptions are mentioned in a footnote (cf. Section 4.4).

5.1.5.2 Test compound

If the tested substance is a metal, the column 'substance purity' is replaced by the column 'test compound'. Toxicity data of metal compounds are always expressed in quantities relating to the element and not as the salt, e.g. mg Co²⁺/l. In most cases tests with metals are performed with pro analysis salts or technical grade salts. If impurities are present, this should be mentioned in a footnote. In the tables the metal species will be mentioned in the column 'test compound', e.g.: CoSO₄.

5.1.6 Test water

In this column, the following test waters are distinguished :

- am artificial media
- nw natural water
- ns natural sea water
- rw reconstituted water
- tw tap water

5.1.7 pH

Data from a study in which a range of pH values is tested, are handled as follows:

- All data are selected, obtained in experiments performed under conditions that fit in the ranges recommended by the OECD guidelines for several species.
- When the tested species is not included in the OECD guidelines, select all data with circumstances in accordance with the natural habitat of the tested species. The geometric mean of these toxicity values will be reported in the table.
- For some compounds it is not possible to calculate the geometric mean because there might be a relation between toxicity and pH. In this case all reported values are presented separate and used in risk assessment. The same procedure is followed for temperature ranges.

5.1.8 Water properties

The following column can be either “hardness” for freshwater toxicity tables, or “salinity” for saltwater toxicity tables.

5.1.8.1 Hardness

Hardness is expressed in German degrees of hardness, with 1 dH = 0.1783 mmol CaCO₃ per liter. The German degree of hardness (dH) can be calculated from other Ca- and Mg-compounds following formula (27):

$$dH = (2x \text{ mmol } Ca^{2+} + 2y \text{ mmol } Mg^{2+}) * 2.8 \quad (27)$$

Molecular weights for often-used recalculations are:

Ca	= 40.1	Mg	= 24.3
CaCO ₃	= 100.1	MgSO ₄	= 120.4
CaSO ₄	= 136.1	Mg(NO ₃) ₂	= 148.3
Ca(NO ₃) ₂	= 164.1		
CaCl ₂	= 111.0		

5.1.8.2 Salinity

The salinity is expressed as ‰ (ppt). Water with a salinity of at least 20 promille is qualified as marine water. Freshwater has salinity of 5 promille or less, brackish water between 5 and 20 promille. The category “brackish” is not represented in separate tables. Animals belonging to this category are included in the saltwater tables.

5.1.9 Exposure time

In this column, exposure time is expressed as:

- months (m); (>19 w in months, 1 month = 4.3 weeks)
- weeks (w); (5-19 w)
- days (d); (5-31 d)
- hours (h); (1-96 h)
- minutes (min); (0-60 min)

Whether data are categorised as chronic or acute toxicity data depends on the criteria listed in Section 4.3. For a number of species from several taxonomic groups the OECD has set up a number of standard fixed test durations. The length of these standard test durations can be found in the OECD guidelines for testing of chemicals. In addition to these guidelines, specific guidelines are available for the purpose of deriving ERLs (Section 4.3).

5.1.10 Test criterion

The test criterion is preferably expressed as acute L(E)C50 or chronic NOEC. Only those effect parameters are taken into account that affect the species on the population level, as discussed under heading 4.3.1, 'preferred endpoints'. Whether other effect parameters, e.g. behaviour, are included in the tables is decided in each individual case and is reported in a footnote.

5.1.11 Ecotoxicological endpoint

In this column, the endpoints are specified briefly. The most common ones are:

- Growth growth
- Repro reproduction
- Mort mortality
- Immo immobilisation
- Morpho morphological effects
- Hist histopathological effects

Growth and reproduction endpoints are exactly specified in a table note, e.g. reproduction measured as number of eggs.

Test result and derivation of L(E)C50/NOEC

Test results or effect concentrations are reported in this column in mg/l or µg/l. The toxicity data are rounded off to maximally two significant digits, by rounding off 1 to 4 downwards, and 5 to 9 upwards (e.g. 2035 becomes 2000 and 1.485 becomes 1.5).

When more than one result is obtained under identical circumstances in the same test from the same laboratory (e.g. the same test with hardness 40 and 70) the geometric mean of the results will be reported in the table. In some cases however, it is better to report the values separately for the 'weight of evidence' approach (e.g. two temperatures both relevant in the field for the species used. The lowest value predicts a conceivable situation in field situations).

5.1.11.1 L(E)C50 values

L(E)C50 values are reported as such. If only raw data are available the L(E)C50 is calculated according to the method of Spearman and Karber (Hamilton et al., 1977). This method is used only when the test parameter is mortality and immobility and is mentioned in the footnote. When data for calculation are lacking or could not be fitted, the \leq or \geq L(E)C50 values are reported in a separate table 'Toxicity data from deviating tests'.

5.1.11.2 NOEC values

NOEC values for aquatic organisms are derived using the procedure under heading 4.4, 'Data selection and treatment'.

If a NOEC is derived from a LOEC, the effect percentage observed at the LOEC and the factor applied are mentioned in a footnote. When sufficient data for calculation are lacking, the \leq or \geq NOEC values are reported in a separate table 'Toxicity data from deviating tests'.

5.1.12 Notes

This column contains the footnote numbers that are listed below the toxicity tables.

5.1.13 Reference

This column lists the reference to the study. All studies that are mentioned in the tables, including those mentioned in the deviating tables, are placed in the reference list. Data originating from CSR summaries are referred to as "RIVM/CSR archives, (year)". If a study is not valid according to the outlined methods, the study will be placed in the second part of the reference list called "evaluated but rejected".

5.2 Soil toxicity data

This section concerns tables for toxicity to soil organisms, microbial processes and enzymatic activity. Examples of standardised soil toxicity tables are given in Annex 3B. The column entries in the toxicity tables are discussed below. Soil toxicity data are subdivided and tabulated as

- Chronic toxicity to soil organisms
- Acute toxicity to soil organisms
- Microbial processes and enzymatic activity
- Toxicity data from deviating tests

5.2.1 Species/process/activity

Data for species and processes are not combined but are evaluated separately as elaborated in Section 4.4. This column can either contain microbial processes, enzyme activity or soil species.

5.2.1.1 Microbial processes/enzyme activities

Enzyme activities of microorganisms, such as amylase, phosphatase and dehydrogenase etc. are listed as process. More general microbial activities or functions are listed as respiration, nitrification, ammonification, sulphur oxidation etc.

5.2.1.2 Species

Proposed taxonomic classification groups of soil organisms are listed in Table 13. The species name should be mentioned in the table, and listed under the correct taxonomic group (Annex 3B). The main taxons encountered are shown in Table 13.

5.2.2 Species properties

This column can be empty for microbial processes and enzymatic activity and can then be omitted. In other cases, age, size, weight or lifestage is mentioned, following the name of the organism. The toxicity data of animals with different age, size or weight are presented individually in the tables. When the tested organisms are

collected from field populations, this fact is mentioned in a footnote with the duration of the acclimation period. When the authors report that the organisms are originating from a contaminated area the test is not included.

Table 13: Taxonomic classification of soil organisms

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

5.2.3 Soil type

This column lists the soil type, e.g. sandy loam or clay. If percentages of clay, sand and loam are given, the soil type can be derived with the American Soil Classification System (see Annex 4).

5.2.4 pH

pH values in pH-KCl are preferred. In the footnotes is mentioned whether the pH is measured as: pH-KCl, pH-H₂O or unknown.

5.2.5 % organic matter (% OM)

If in a study the percentage organic carbon is given, recalculation to percentage organic matter (OM) is necessary according to:

$$\%OM = \%OC \times 1.7 \quad (28)$$

with % OM = percentage organic matter
 % OC = percentage organic carbon

5.2.6 % clay

The % clay (lutum) is used to convert test results for metals to standard soil (see section 4.4.2.1)

5.2.7 Temperature

No criteria have been established.

5.2.8 Exposure time

Exposure time is expressed as:

- months(m); (>19 w in months, 1 month = 4.3 weeks)
- weeks(w); (5-19 w)
- days(d); (5-31 d)
- hours(h); (1-96 h)
- minutes(min); (0-60 min)

Acute toxicity: in view of the life span of the species this will always represent a relatively short period of time, which is species dependent.

Chronic toxicity: this represents a complete or partial life cycle including sensitive young stages or one or more reproduction cycles, the exact length of the time period is species dependent.

In the field of soil toxicity a strict definition of exact acute and chronic test duration is lacking. In the OECD guidelines fixed test durations are mentioned only for earthworms (a 14 days acute test to derive the LC50, a chronic reproduction earthworm test is still in development at OECD) and macrophytes (an EC50 early life stage growth test and an LC50 emergence test). Because of this lack of information it is decided case by case whether a test is acute or chronic.

5.2.9 Test criterion

The test criterion is preferably expressed as acute L(E)C50 or chronic NOEC.

5.2.10 Ecotoxicological Endpoint

Only those effect parameters are taken into account that affect the species on the population level, as discussed under heading 4.3.1, 'preferred endpoints'. Whether other effect parameters, e.g. behaviour, are included in the tables is decided in each individual case and are reported in a footnote.

5.2.11 Result test soil

Effect concentrations are tabulated as mg/kg soil (dry weight). When concentrations have been analysed during the test, the results are expressed as the measured values and indicated with an α placed in the 'Notes' column. Mean concentrations are calculated analogous to the methods applied for static aquatic studies (section 5.1.3).

Soil toxicity studies, especially studies with microorganisms are difficult to interpret. In general each significant inhibition of a microbial process ($P < 0.05$) is considered to be an effect, even when this inhibition disappears in time. Stimulation of microbial processes is in principle not considered to be an adverse effect and is not included in the toxicity tables. Only if the effect can be related to stress of the organism in question (e.g. for Bacteria, a constant population size is observed with a concentration-related increase of oxygen) an ECx or NOEC can be obtained.

When bacteria or fungi are tested according to the "plate count method" these organisms are cultivated on an agar plate after exposure to the toxicant in soil. This method is rather inaccurate and differences between the control and test concentrations up to 30% are not considered to be effects (e.g. EC28 = NOEC). In contrast with the plate count method effects on enzymatic activity can be measured very accurately. In these studies it is possible to determine an EC2 differing significantly from the control value. The values \leq EC10 in these studies are considered to be the NOEC.

In terrestrial ecotoxicology microbial processes are often studied. With pesticides, 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 (Haanstra et al., 1985; Van Beelen et al., 1991). The EC10-value obtained is considered to be the NOEC. Prerequisite is that these ECs 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. If only one EC is available in the original study this EC is converted to a NOEC according to Section 4.4.1.

Calculation of the Predicted Initial Environmental Concentration (PIEC)

If in a laboratory study field doses are expressed as kg a.i./ha or l a.i./ha (a.i. = active ingredient, commonly used for pesticides), one should recalculate this value into the PIEC which is expressed in mg a.i./kg. For this calculation a number of default values have been established (Emans et al., 1992). To establish these default values it is assumed that granules, if mixed with the soil, are distributed homogeneously over the top 20 cm of soil. If granules or sprays are not mixed, a distribution over the top 5 cm is assumed for calculation of the PIEC. The soil is assumed to have a bulk density of 1400 kg/m³ (eqn. 29). The PIEC is considered to be equal to the concentration on day 0. If a field dose is expressed as [l a.i./ha] one should use the specific gravity of the compound to recalculate this value to [kg a.i./ha]. The calculation of the PIEC should be mentioned in the footnote and is performed as

$$PIEC = \frac{Dose * mgPkg}{m2Pha * H_{soil} * B_d} \quad (29)$$

with:	PIEC	= predicted initial env. Concentration [mg a.i./ kg soil]
	Dose	= [kg a.i./ha]
	MgPkg	= 1.10 ⁶ [mg/kg]
	M2Pha	= 1.10 ⁴ [m2/ha]
	H _{soil}	= soil depth, if mixed: 0.2 [m] = soil depth if not mixed: 0.05 [m]
	B _d	= bulk density: 1400 [kg/m ³]

5.2.12 Result standardised soil/sediment

Tests performed on different soils or with different sediments, as reported in the preceding column of the data table, are standardised by conversion to a standard soil or sediment as described in Section 4.4.2. The standardised data are reported in this column. The type of standard soil may differ in the framework of pesticide registration. The type of standard soil should be reported in a footnote.

5.2.13 Notes

This column contains the footnote numbers that are listed below the toxicity tables. If the purity of the tested substance is known, it is included in the notes. The purity of the tested substances is dealt with as described for aquatic studies (Section 5.1.5).

5.2.14 Reference

This column lists the reference to the study. All studies that are mentioned in the tables, including those mentioned in the deviating tables, are placed in the reference

list. Data originating from studies summarised by RIVM/CSR are referred to as 'RIVM/CSR archives, (year)'. If a study is not valid according to the outlined methods, the study will be placed in the second part of the reference list called 'evaluated but rejected'.

5.3 Bird and mammal toxicity data

In order to assess possible effects due to secondary poisoning toxicity studies for birds and mammals are evaluated: subacute and (semi)chronic studies with mammals and acute and (semi)chronic studies for birds, all exposed via food. LC50 values for birds and NOEC values are derived. Relevant OECD guidelines are 205, 206, 407/409, 414/416, 451/453. Examples of a standardised toxicity table for birds and mammals are given in Annex 3E.

5.3.1 Species

The species name should be mentioned in the table.

5.3.2 Species properties

If available, age, size, weight or lifestage is mentioned, with the sex (if known) between brackets. The toxicity data of animals with different age, size or weight are presented individually in the tables (if available).

5.3.3 Substance purity

The substance purity is reported, cf. section 5.1.5.

5.3.4 Application route

This column reports the route of application, such as gavage (oral dosage), diet, water etc.

5.3.5 Exposure time

The exposure time is reported in months, days, hours or minutes cf. section 5.1.9.

5.3.6 Test criterion.

The test criterion is mentioned (cf. Section 4.3 and 5.1.10.). The term acute LC50 is used only to denominate acute oral LD50 tests.

5.3.7 Ecotoxicological Endpoint

The endpoint most frequently encountered will be mortality, but occasionally, other endpoints may be used and recorded in this column.

5.3.8 Effect concentration gavage

Gavage dosing concentrations are reported in $\text{mg.kg bw}^{-1}.\text{d}^{-1}$. These concentrations are recalculated and reported as well in the next column, using the conversion factors from table 11 in Section 4.4.6.

5.3.9 Effect concentration diet

This column shows effect concentrations from diet studies (in mg/kg food) or recalculated effect concentrations from gavage dosing studies.

5.3.10 Notes

This column contains the footnote numbers. Footnotes contain specific study details or additional remarks.

5.3.11 Reference

This column lists the reference to the study. All studies mentioned in the tables, including those mentioned in the deviating tables, are placed in the reference list. If data are taken from previous studies, reviews or compilations, the original source should preferably be mentioned. Data originating from CSR summaries are referred to as 'RIVM/CSR archives, (year)'.

5.4 Partition coefficients

When partition coefficients are calculated or taken from several studies, they can be documented in a separate table. An example of a standardised partition coefficient table is given in Annex 3C.

5.4.1 Test substance

The name of the test substance is reported here (with the purity between brackets).

5.4.2 Substance purity

See section 5.1.5

5.4.3 Soil type

See Section 5.2.3

5.4.4 Organic carbon content

This column records the organic carbon content as a percentage.

5.4.5 pH

See Section 5.2.4

5.4.6 Cation exchange capacity (CEC)

The CEC (expressed in mmol/kg) is an indication for the potential of the soil to adsorb cations on the surface of soil solid particles. Adsorption processes are reversible; desorption of a ion occurs after adsorption of another ion, the ions are exchanged.

5.4.7 Solid/water mass distribution (g/l)

Solid/water concentrations should be chosen in such a way that adsorption will lie between 20 to 80%. Studies with experimental conditions resulting in nearly complete or no adsorption are excluded from the table.

5.4.8 Mass balance

Is the concentration of the chemical after equilibrium determined in both the water and soil, allow calculation of a mass balance: Y. Is the concentration of the chemical determined in the water only: N

5.4.9 Equilibration time

Equilibration time is expressed in hours. To determine the period required for equilibration of the adsorption process, the progress of the adsorption should be determined (in a preliminary experiment). If possible check whether equilibrium is reached or not.

5.4.10 Log K_{oc}

When for one substance several log K_{oc} values are available, the median value is calculated.

5.4.11 Notes

This column contains the footnote numbers. Footnotes contain specific study details or additional remarks.

5.4.12 Reference

This column lists the reference to the study. All studies mentioned in the tables, including those mentioned in the deviating tables, are placed in the reference list (cf. section 5.3.11).

5.5 BCFs or BSAFs

When bioconcentration factors (BCFs) and or biota to soil or sediment accumulation factors (BSAFs) are calculated or taken from several studies, they are documented in separate tables. An example of a BCF table is presented in Annex 3D.

5.5.1 Species

The species name should be mentioned in the table.

5.5.2 Species properties

If available, age, size, weight or lifestage is mentioned, with the sex (if known) between brackets. The toxicity data of animals with different age, size or weight are presented individually in the tables (if available).

5.5.3 Test type

The test types are reported, as distinguished as in section 5.1.4.

5.5.4 Substance purity

See section 5.1.5

5.5.5 Test water

In this column, test waters are reported as distinguished in section 5.1.6.

5.5.6 pH

pH is reported, as described in section 5.1.7.

5.5.7 Water properties

The following column can be either 'hardness' for freshwater toxicity tables, or 'salinity' for saltwater toxicity tables.

5.5.7.1 Hardness

Hardness is expressed as mg CaCO₃ per litre as described in section 5.1.8.

5.5.7.2 Salinity

The salinity is expressed as ‰ (ppt), cf. section 5.1.8.

5.5.8 Exposure time

In this column, exposure time is expressed as listed before in section 5.1.9.

5.5.9 Exposure concentration

In this column, exposure concentrations are recorded.

5.5.10 Time to Equilibrium

The time needed to establish or estimate equilibrium in the organism is recorded in this column, if available

5.5.11 Dry to wet weight ratio

The fraction dry to wet weight is recorded to facilitate wet to dry weight conversion (cf. Section 4.4.6) or vice versa. If original data on dw/ww ratio's are reported, these are preferred over generic dw/ww ratios.

5.5.12 BCF/BSAF

The BCF (for aquatic organisms) or BSAF (for soil or sediment organism) is shown. Correct units of the BCF or BSAF are crucial and should always be checked before reporting.

5.5.13 Notes

Footnote numbers are listed referring to additional study details. If only BSAFs are reported, they may be recalculated to BCFs using equation 14. The concentration suspended solids is input in this equation and is reported in a note.

5.5.14 Reference

This column lists the reference to the study. If data are taken from previous studies, reviews or compilations, the original source should preferably be mentioned.

5.6 ERLs

The ERLs, shown in the results and in the (extended) summary are reported as Negligible Concentration (NC), Maximum Permissible Concentration (MPC) and as Serious Risk Concentration for ecosystems (SRC_{ECO}) in the appropriate units (µg/l or mg/kg dry soil). In principle, they are reported for water, soil and sediment (Table 14). Groundwater ERLs are only reported for the SRC_{ECO}. In the case of secondary poisoning (SP), ERLs are reported for separate SP data, separate direct toxicity data and combined data (cf. Smit et al., 2000). Total concentrations in freshwater or marine water are based on a concentration of 30 mg/l suspended matter. Calculations are elaborated in Annex 10.

Table 14: Overview of reported ERLs by compartment.

Compartment	Phase	Reported ERLs ‡
Freshwater	Dissolved Total*	NC/MPC/SRC _{ECO} NC/MPC/SRC _{ECO}
Marine water	Dissolved Total*	NC/MPC/SRC _{ECO} NC/MPC/SRC _{ECO}
Groundwater	Dissolved	NC/MPC/SRC _{ECO}
Soil	Standard soil **	NC/SRC _{ECO}
Sediment	Standard sediment **	NC/MPC/SRC _{ECO}
Air		NC/MPC

‡ only if not calculated before and data availability allows calculation

* Based on 30 mg/l suspended matter (cf. Annex 10)

** with 10 % organic matter and 25 % clay

6. Calculating Environmental Risk Limits

The extrapolation methods that are used for hazard assessment¹, and also for deriving the Environmental Risk Limits, are the ‘Refined effect assessment’ (Section 6.1), and the ‘Preliminary effect assessment¹’ (Section 6.2). The former method, based on species sensitivity distributions, is preferred over the latter and applied if chronic toxicity data for 4 or more different taxonomic groups are available. The latter method is applied if chronic data for less than 4 species of different taxonomic groups, less than 4 data on different processes or only acute data are available.

For naturally occurring substances, such as metals, the ‘Added Risk Approach’ is applied (Section 6.3). For both organic substances and metals that potentially accumulate through the foodchain, ERLs are derived combining direct toxicity and secondary poisoning as described in Section 6.4. In case insufficient toxicity data are available for soil or sediment, ERLs are derived based on aquatic toxicity data and applying the Equilibrium Partitioning Method (Section 6.5).

Independently derived ERLs have to be harmonised with those for water. The final harmonisation of ERLs is discussed in Section 6.6.

Probabilistic modeling is recently used for PCBs (Van Wezel et al, 2000), but this procedure is not ratified yet by the scientific steering committee for ERLs (Stuurgroep INS) and is currently under review by scientific advisory councils. This procedure is devised for substances that accumulate through the foodchain and is discussed in Annex 7. ERLs are documented in the final report (Annex 9). Derived ERLs are compared to multi-species (semi) field experiments and monitoring data (if available), to establish the validity of ERLs for the protection of ecosystems.

6.1 Refined effect assessment

6.1.1 Introduction

It is recognized that living organisms represent a vast array of taxonomic diversity, life histories, physiologies, morphologies, behaviours and geographical distributions. For ecotoxicology, these biological differences mean that different species respond differently to a compound at a given concentration (i.e., different species have different sensitivities). The acknowledgement that species sensitivities to toxic compounds differ (without attempting to explain the cause), and describing that variation with a statistical distribution function yields Species Sensitivity Distributions (SSDs) as introduced by Stephan et al. (1985) and Kooijman (1987). The basic assumption of the refined effect assessment or statistical extrapolation method is that the log of the sensitivities of a set of species in a community can be described by some distribution, usually a parametric distribution function such as the normal or logistic distribution. The available ecotoxicological data are seen as a sample from this distribution and are used to estimate the parameters of the Species Sensitivity Distribution. The variance in sensitivity among the test species and the

¹ The derivation of environmental risk limits can be viewed as a generic hazard assessment approach. The use of the term ‘effect assessment’ is mainly for historical reasons and association with policy terms.

mean are used to calculate a concentration that can be used as an environmental risk limit (ERL). Specific percentiles of the SSD are chosen to determine ERLs such as the MPC and the SRC_{ECO} (section 6.1.2). For risk assessment purposes, the SSD can also be used to estimate the potentially affected fraction of species (PAF); species likely to be exposed above the toxicological endpoint in the analysis (in this case, NOECs). The current statistical extrapolation method assumes that the log-transformed NOECs that are used for estimating the distribution fit the normal distribution. Deviations from normality are a trigger for further analysis.

The method is applied provided that at least 4 NOEC values of species of different taxonomic groups are available¹. For a detailed overview of the theory and the statistical adjustments since its introduction, it is referred to the original literature (Kooijman, 1987; Van Straalen and Denneman, 1989; Wagner and Løkke, 1991, Aldenberg and Slob, 1993; Aldenberg and Jaworska, 2000, Posthuma et al., in prep).

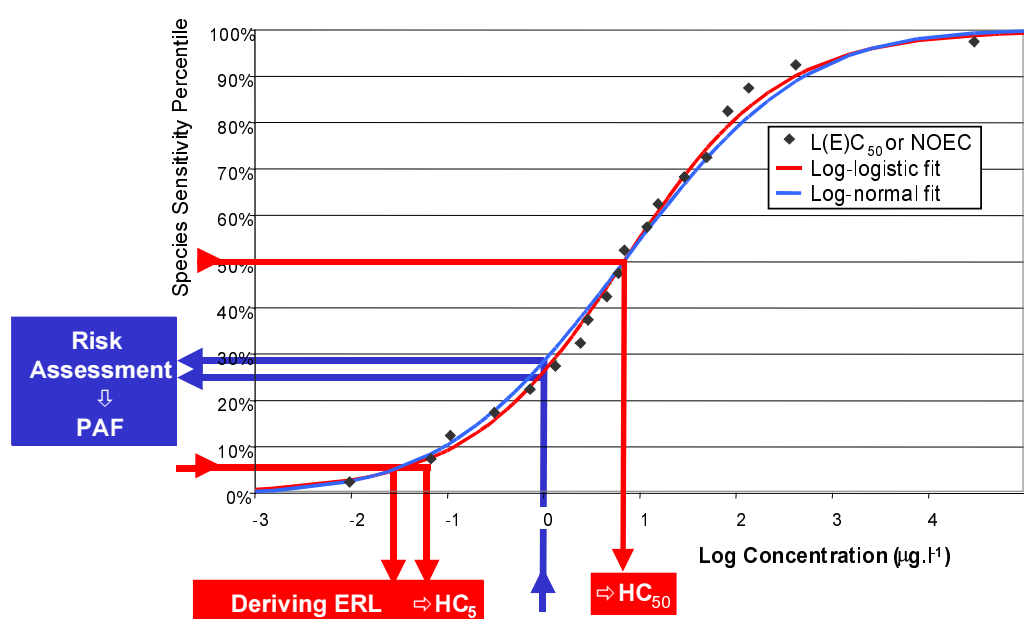


Figure 4: Species Sensitivity Distributions used to derive ERLs or to calculate the potentially affected fraction (PAF). Dots are input data, the line is the fitted SSD. Inverse use: ERLs at a certain cut-off value (here, the 5th and 50th percentile). Forward use: risk assesment.

Until mid-2000, the statistical extrapolation method of Aldenberg and Slob (1993) was used for derivation of ERLs with the use of SSDs (cf. Crommentuijn et al., 2000b,c). This method, based on the log-logistic fit is now replaced in favour of the method of Aldenberg and Jaworska (2000). The difference between the methods is that the use of the logistic distribution of log-transformed toxicity data is now replaced by a normal distribution of log-toxicity data. The differences between these two distributions are small and are mainly noticeable in the tails of the distribution (cf. Figure 4). At small sample size, as is usually the case for deriving ERLs, there is no statistical or theoretical justification for choosing the logistic or normal distribution (Aldenberg and Jaworska, 2000). The advantage of analytical tractability of the

¹ A recent EU workshop in London discussed the minimum number of species and which taxa to include (ECB, 2001). This discussion has not yet been resolved.

logistic distribution is outweighed by the statistical advantage of using the normal distribution of log-toxicity data. Based on the concept of tolerance limits in quality control (Odeh and Owen, 1980), normal distribution theory provides the methods to calculate confidence intervals.

6.1.2 Deriving ERLs

ERLs can be derived using SSDs based on the selected NOEC values, where the MPC is estimated from the 5th percentile of the SSD, the HC₅ and the SRC_{eco} is estimated from the 50th percentile or median of the SSD, the HC₅₀.

Since it is now possible to routinely calculate confidence intervals, the 90% confidence interval of the HC₅ and HC₅₀ values and the confidence interval of the percentage of species potentially affected at a given environmental concentration, the PAF, are reported as well (cf. Verbruggen et al, 2000).

The current method to calculate the HC₅ and HC₅₀ makes use of the log-normal species sensitivity distribution (Aldenberg and Jaworska, 2000) instead of a log-logistic distribution. The HC₅ and HC₅₀ are calculated as (Aldenberg and Jaworska, 2000):

$$\log HC_p = \bar{x} - k \cdot s \quad (29)$$

with

HC_p = Hazardous concentration for p% of the species, with HC5 for the MPC and HC50 for the SRC_{ECO}.

\bar{x} = mean of log-transformed NOEC data

k = extrapolation constant depending on protection level and sample size (Table 1 from Aldenberg and Jaworska, 2000, cf Annex 6)

s = standard deviation of log-transformed data.

Extrapolation constant *k* is taken from Table 1 of Aldenberg and Jaworska (Annex 6). It should be noted that the *median* estimate of the HC5 and the HC50 are the advised ERLs, and that the 90% confidence intervals are calculated using the lower and upper extrapolation factors from Annex 6. Since the HC50 is simply the median value of the SSD, it is equal to \bar{x} , the mean of log-transformed NOEC data (i.e. *k* = 0). The lower and upper extrapolation factors for the HC50 are taken from Annex 6. Software is available at RIVM to calculate the ERLs from the selected (NOEC) toxicity data based on Aldenberg and Jaworska (2000).

The method of Aldenberg and Jaworska (2000) is used for deriving the SRC_{ECO} and MPC if NOECs for four or more different taxonomic groups are available. For aquatic species, freshwater and marine data are combined if there are no differences in sensitivity between these groups. This is tested with an unpaired, two –sided T-test¹. Prior to this, differences in variance are tested by an F-test. If significant differences in variance are observed, the unpaired T-test is performed with a Welch correction for differences in variance. When there is a statistically significant difference, distributions for freshwater and marine species are estimated separately.

¹ With a significance level alpha=0.05.

For toxicants with a specific toxic mode of action, specific sensitive taxonomic group(s) may be found, belonging to the target species. If prior knowledge about sensitive (target) species is available, a statistical analysis should be performed for confirmation or rejection of the different sensitivities of the groups¹.

When NOEC values calculated from toxicity experiments with birds or mammals are available (if a substance meets the criteria of Table 3, cf. Section 4.4.6), these NOECs are added to the NOECs for direct toxicity and are used as input to this method.

The final NOEC data set is tested for deviations from a Gaussian distribution using the Kolmogorov-Smirnov test where the mean and SD are estimated from the sample of NOEC data. It should be realized that this test has limited validity if the sample contains less than a dozen values. Small sample sizes do not provide enough data to discriminate between Gaussian and nongaussian distributions. If the P value is large², and the sample size is small, this only means that the data are not inconsistent with a Gaussian population. This does not exclude the possibility of a nongaussian population. If a data set has less than four values, it is impossible to test normality.

The Negligible Concentration (NC) is not based on a specific protection criterion derived from an SSD, but is based on a safety factor for combination toxicity (VROM 1989a,b). The NC is derived from the MPC by dividing it by a factor of 100.

The end result of the refined effect assessment using SSDs is an MPC and an SRC_{ECO} with reported 90% confidence intervals, and an NC derived from the MPC for each environmental compartment. In case of secondary poisoning, see Section 6.3 for details.

6.2 Preliminary Effect Assessment

If chronic NOECs are available for less than 4 taxonomic groups, preliminary risk assessment is applied. The preliminary effect assessment method is a method in which assessment factors are applied to the selected chronic or acute toxicity data. The size of this factor depends on the number and kind of these toxicity data.

Tables 15 to 17 show the assessment factors of the Technical Guidance Document (TGD) for deriving the Predicted No-Effect Concentration (PNEC), which is similar to the MPC, for water, soil and secondary poisoning (ECB, 1996). Since 1999, the latter assessment factors are primarily used to derive MPCs for water and soil (Kalf et al., 1999). In many cases, the number of available ecotoxicological data does not meet the conditions for application of the assessment factors from the TGD. In that case, the modified EPA assessment factors are used (Kalf et al., 1999). For exposure to volatile substances in air, the modified EPA assessment is used since the TGD does not provide guidance. Tables 18 to 20 list these assessment factors for aquatic MPCs, terrestrial MPCs, secondary poisoning MPCs and air MPCs, respectively. The Negligible Concentration (NC) is not based on a specific protection criterion, but is

¹ Although not ratified by scientific advisory groups, separate SSDs could be fitted and ERLs could be reported for separate and combined data sets as described in sections 4.4.2 and 4.5.1.1 (cf. Van Wezel and Van Vlaardingen, 2000).

² The P value (as reported by GraphPad Prism, 1996) for Dallal and Wilkinson's approximation to Lilliefors' method (Am. Statistician, 40:294-296, 1986).

based on a safety factor for combination toxicity (VROM 1989a,b). The NC is derived from the MPC by dividing it by a factor of 100. The factors and conditions used for deriving the SRC_{ECO} in the preliminary risk assessment method are shown in Table 22.

6.2.1 TGD/EU factors

It was decided to use the assessment factors from the Technical Guidance Document of the European Union (ECB, 1996), because of the harmonisation of the project 'Setting Integrated Environmental Quality Standards' with the framework of admission of plant protection products and biocides (Kalf et al., 1999). Some modifications have been applied to the original TGD schemes for the purpose of the project 'Setting Integrated Environmental Quality Standards'.

- First, the classification in taxonomic groups is used instead of the original classification in trophic levels, because this classification is used throughout the whole derivation of MPCs.
- Second, for terrestrial data a comparison with the MPC derived with equilibrium partitioning is made in all cases of preliminary risk assessment.
- A third modification is that for the geometric mean of several toxicity data for one species is taken, if based on the same toxicological endpoint, instead of the arithmetic mean.

Table 15. EU/TGD assessment factors for aquatic organisms.

Available data	Additional criteria	MPC based on	Assessment factor
L(E)C50s for algae, Daphnia and fish (base set)		$L(E)C50_{aqua_{min}}$	1000
Base set + 1 NOEC (not algae)	NOEC from same taxonomic group as $L(E)C50_{aqua_{min}}$ (fish or Daphnia)?		
	Yes	$NOEC_{aqua_{min}}$	100
	No: $L(E)C50_{aqua_{min}}/1000 < NOEC_{aqua_{min}}/100$	$L(E)C50_{aqua_{min}}$	1000
	No: $L(E)C50_{aqua_{min}}/1000 \geq NOEC_{aqua_{min}}/100$	$NOEC_{aqua_{min}}$	100
Base set + 2 NOECs	NOEC from same taxonomic group as $L(E)C50_{aqua_{min}}$?		
	Yes	$NOEC_{aqua_{min}}$	50
	No	$NOEC_{aqua_{min}}$	100
Base set + 3 NOECs	NOECs for algae, Daphnia and fish?		
	Yes	$NOEC_{aqua_{min}}$	10
	No: NOEC from same taxonomic group as $L(E)C50_{aqua_{min}}$	$NOEC_{aqua_{min}}$	10
	No: NOEC not from same taxonomic group as $L(E)C50_{aqua_{min}}$	$NOEC_{aqua_{min}}$	50

Completeness of the base set is required for the aquatic compartment, i.e. acute toxicity studies for algae, *Daphnia* and fish. However, for more hydrophobic compounds (acc. to the TGD, with $\log K_{ow} \geq 3$) short term toxicity data may not be representative, since the time span of an acute test may be too short to reach a toxic internal level. In those cases, the completeness of the base set is not demanded and an assessment factor of 100 may be applied to a chronic test, which should not be an alga test if this is the only chronic test available. This result should still be compared to the

outcome of assessment factors applied to LC50 values. Intermittent release is not relevant for derivation of MPCs and therefore, this item is omitted from table 15.

When the base set is incomplete and the TGD table can not be applied, the modified EPA method should be used. According to the EPA method an assessment factor of only 10 should be applied to the lowest NOEC, while the highest assessment factor in the EU/TGD method to apply to a chronic NOEC, if the base set is complete, is 100. To eliminate this inconsistency when the base set is incomplete, a factor 100 and/or 1000 will be applied to the lowest NOEC and/or L(E)C50, respectively, to derive the MPC.

Toxicity data for birds and mammals are usually available as LC50s (e.g. 5 days dietary study with birds) or NEC values (e.g. 28 days oral study with rats). If results are expressed in mg/kg body weight they should be converted to mg/kg food using the conversion factors of Table 11. Toxicity data reported in mg/kg food are converted to concentrations in water, soil or sediment using eqns. 15-18 (Section 4.4).

Table 16. EU/TGD assessment factors for terrestrial species/processes.

Available data	Additional criteria	MPC based on	Assessment Factor
≥ 1 L(E)C50		L(E)C50 _{terr.min}	1000
1 NOEC, no L(E)C50s		NOEC _{terr.min}	100
1 NOEC, ≥ 1 L(E)C50s	$L(E)C50_{terr.min}/1000 < NOEC_{terr.min}/100$	L(E)C50 _{terr.min}	1000
	$L(E)C50_{terr.min}/1000 \geq NOEC_{terr.min}/100$	NOEC _{terr.min}	100
2 NOECs	NOEC from same taxonomic group as L(E)C50 _{terr.min} ?		
	Yes	NOEC _{terr.min}	50
	No	NOEC _{terr.min}	100
3 NOECs	NOEC from same taxonomic group as L(E)C50 _{terr.min} ?		
	Yes	NOEC _{terr.min}	10
	No	NOEC _{terr.min}	50

The rules for the use of assessment factors when extrapolating bird and mammal toxicity are different between the modified EPA method and the EU/TGD method (ECB, 1996, p. 350-351). Table 17 lists the data requirements and criteria for application of the EU/TGD assessment factors. Additional criteria are drafted to compare the available acute and chronic data. When these factors cannot be applied, the EPA table for birds and mammals should be used (Table 20).

Acute LD50 studies on rats or birds are not extrapolated to a chronic value as these tests are not dietary tests. The EU/TGD considers NOECs from reproduction studies to be equal to chronic studies (yielding an assessment factor of 10), but test duration must be sufficiently long to allow proper evaluation of reproduction effects. The EU guidelines are more strict in the evaluation of acute data since the EPA's assessment factor of 100 for at least three L(E)C50 values (Table 20) is not allowed.

Table 17 EU/TGD assessment factors for birds and mammals

Available data	Additional criteria	MPC based on	Assessment Factor
≥ 1 LC50	Usually dietary tests of 5 days	$L(E)C50_{min}$	1000
≥ 1 NOEC 28 days test	$NOEC_{min}/100 \leq L(E)C50_{min}/1000$ $NOEC_{min}/100 > L(E)C50_{min}/1000$	$NOEC_{min}$ $L(E)C50_{min}$	100 1000
≥ 1 NOEC 90 days test	$NOEC_{min}/30 \leq L(E)C50_{min}/1000$ $NOEC_{min}/30 > L(E)C50_{min}/1000$	$NOEC_{min}$ $L(E)C50_{min}$	30 1000
≥ 1 NOEC chronic (> 90 days)	$NOEC_{min}/10 \leq L(E)C50_{min}/1000$ $NOEC_{min}/10 > L(E)C50_{min}/1000$	$NOEC_{min}$ $L(E)C50_{min}$	10 1000

6.2.2 Modified EPA assessment factors

When the base set is incomplete and the TGD tables can not be applied, the modified EPA method should be used for deriving ERLs (Van de Meent et al., 1990). Assessment factors for exposure to substances in air are not available in the EU guidance, and the EPA factors are used. The factors and conditions used in this method for deriving MPCs from aquatic, terrestrial and air exposure studies and for secondary poisoning are shown in Tables 18-21, respectively. The use of quantitative structure-activity relationships (QSARs) is allowed within the validity domain of the QSARs (Annex 8). If data are available for terrestrial species as well as processes, the data are considered separately and ERLs are derived for both.

Table 18. Modified EPA assessment factors for aquatic organisms.

available data	Additional criteria	MPC based on	Assessment Factor
$L(E)C50$ or QSAR estimate	$L(E)C50_{aqua_{min}}/1000 < NOEC_{aqua_{min}}/10$	$L(E)C50_{aqua_{min}}$	1000
$L(E)C50$ or QSAR estimate for minimal algae/crustaceans/fish	$L(E)C50_{aqua_{min}}/100 < NOEC_{aqua_{min}}/10$	$L(E)C50_{aqua_{min}}$	100
NOEC or QSAR estimate **	$L(E)C50_{aqua_{min}}/1000 (100) < NOEC_{aqua_{min}}/10$	$L(E)C50_{aqua_{min}}$	100/1000
	$L(E)C50_{aqua_{min}}/1000 (100) \geq NOEC_{aqua_{min}}/10$	$NOEC_{aqua_{min}}$	10
NOEC or QSAR estimate for minimal algae/crustaceans/fish		$NOEC_{aqua_{min}}$	10

** The value based on NOECs is compared to the extrapolated value based on acute $L(E)C50$ toxicity values. The assessment factor for $L(E)C50$ s is 100 for $<3 L(E)C50$ s, 1000 $\geq 3 L(E)C50$ s.

Table 19. Modified EPA assessment factors for terrestrial organisms.

available data	Additional criteria	MPC based on	Assessment Factor
$L(E)C50$ or QSAR estimate	$L(E)C50_{terr_{min}}/1000 < NOEC_{terr_{min}}/10$	$L(E)C50_{terr_{min}}$	1000
$L(E)C50$ or QSAR estimate for minimal three representatives of microbe-mediated processes, earthworms or arthropods and plants	$L(E)C50_{terr_{min}}/100 < NOEC_{terr_{min}}/10$	$L(E)C50_{terr_{min}}$	100
NOEC or QSAR estimate **	$L(E)C50_{terr_{min}}/1000 (100) < NOEC_{terr_{min}}/10$	$L(E)C50_{terr_{min}}$	100/1000
	$L(E)C50_{terr_{min}}/1000 (100) \geq NOEC_{terr_{min}}/10$	$NOEC_{terr_{min}}$	10
NOEC or QSAR estimate for minimal three representatives of microbe-mediated processes, earthworms or arthropods and plants		$NOEC_{terr_{min}}$	10

** The value based on QSARs is compared to the extrapolated value based on acute $L(E)C50$ toxicity values. The assessment factor for $L(E)C50$ s is 100 for $<3 L(E)C50$ s, 1000 $\geq 3 L(E)C50$ s.

Table 20. Modified EPA assessment factors for bird and mammal toxicity data

available information	Additional criteria	MPC based on	Assessment factor
less than 3 L(E)C50 values	$L(E)C50_{bird_mam_min}/1000 < NOEC_{bird_mam_min}/10$	$L(E)C50_{bird_mam_min}$	1000
at least 3 L(E)C50 values	$L(E)C50_{bird_mam_min}/100 < NOEC_{bird_mam_min}/10$	$L(E)C50_{bird_mam_min}$	100
less than 3 NOECs**	$L(E)C50_{bird_mam_min}/1000 (100) \geq NOEC_{bird_mam_min}/10$	$NOEC_{bird_mam_min}$	10
3 NOECs		$NOEC_{bird_mam_min}$	10

** The value based on NOECs is compared to the extrapolated value based on acute L(E)C50 toxicity values. The assessment factor for L(E)C50s is 100 for <3 L(E)C50s, 1000 ≥ 3 L(E)C50s.

The modified EPA assessment factors for air are to be considered as indicative factors since guidance in this area is virtually lacking (Slooff and Tingey, 1991). They considered mammals, birds, plants, lichens and insects to be representative taxonomic groups for exposure to air pollutants. The assessment factors for air follow the same logic as those for birds and mammals in Table 20.

Table 21. Modified EPA assessment factors for air toxicity data (Slooff and Tingey, 1991).

available information	Additional criteria	MPC based on	Assessment factor
Less than 3 L(E)C50 values and less than 3 NOECs	L(E)C50 may be based on reliable QSAR estimate $L(EC)50/1000 < (NOEC_{min}, n < 3)/10$ (mammal or bird), (plant or lichen), insects	$L(E)C50_{min}$	1000
at least 3 L(E)C50 values and less than 3 NOECs	$L(E)C50_{min}/1000 < (NOEC_{min}, n < 3)/10$. Minimal data set is (mammal or bird), (plant or lichen), insects	$L(E)C50_{min}$	100
less than 3 NOECs**	$L(E)C50_{min}/1000 (100) \geq NOEC_{min}/10$ May be based on reliable QSAR estimate	$NOEC_{min}$	10
≥ 3 NOECs	At least (mammal or bird), (plant or lichen), insects May be based on reliable QSAR estimate	$NOEC_{min}$	10

** The value based on NOECs is compared to the extrapolated value based on acute L(E)C50 toxicity values. The assessment factor is 100 for <3 L(E)C50s, 1000 ≥ 3 L(E)C50s.

6.2.3 Deriving SRC_{ECO}

The factors and conditions used for deriving a SRC_{ECO} in the preliminary risk assessment method are shown in Table 22. In principle, a motivated acute-to-chronic ratio (ACR) is applied the acute toxicity data to compare acute L(E)C50s with chronic NOECs. If no specific information is available, an ACR of 10 can be used. In other cases, the ACR can be derived using existing databases or ACR data specific for a substance.

The ERLs for the terrestrial compartment (derived with the preliminary risk assessment method) are always compared with those derived from the SRC_{eco} for the aquatic compartment by equilibrium partitioning and the lowest is chosen (Section 6.6).

Table 22. Assessment factors used to derive the SRC_{ECO} for the aquatic and terrestrial compartment.

Available data	Additional criteria	SRC_{ECO} based on	Assessment factor
only L(E)C50s and no NOECs		Geometric mean of L(E)C50s	10**
≥ 1 NOECs available	geometric mean of L(E)C50s / 10 < geometric mean of NOECs	Geometric mean of L(E)C50s	10**
	Geometric mean of L(E)C50s / 10 \geq geometric mean of NOECs	Geometric mean of NOECs	1

** An ACR of 10 is used, unless a better estimate is available, e.g. from database analysis.

6.3 Secondary poisoning

Most environmental risk limits are derived from concentrations in water, air, sediment or soil. In the environment some species, in particularly those higher in the foodchain, are additionally or mainly exposed to substances via their food. Through the food, these species may accumulate the potentially toxic substances to high concentrations. This process is called secondary poisoning.

Until 2000, secondary poisoning was assessed by calculating an MPC for secondary poisoning and comparing it to that for direct exposure. Usually, the lowest MPC of the different MPCs calculated is taken as the respective MPC for water or soil (Sijm et al., in prep). This method is now replaced by the alternative method where data for direct exposure and secondary poisoning are combined. Section 4.4.6 discusses the current methods, used for recalculating the NOECs for food exposure to a concentration in water (for aquatic organisms) or soil (terrestrial organisms). New methods have been proposed to refine the assessment of secondary poisoning. The use of probabilistic modeling offers a further tool to do so (Annex 7). Scientific advisory committees have however not yet approved these methods.

Secondary poisoning is generally not taken into account in deriving SR_{ECO} values for soil, since it was decided that for the purpose of the Intervention Values, i.e. pollution at local sites, the geographic areas of interest are too small with regard to protection of ecosystems. Secondary poisoning may be a problem for substantial surface areas of polluted sediment and could be included in future guidance¹

In the case of secondary poisoning, three different HC_5 values ² are reported if refined effects assessment is applied (Smit et al., 2000): one for the combined data set (combined), one for secondary poisoning (SP) based on the bird and mammal toxicity data, and one for the direct toxicity data only (direct). The HC_5 for the combined data set is the recommended MPC; the other HC_5 values are reported for the sake of comparison. MPCs can also be based on preliminary effect assessment, depending on the number and quality of toxicity data.

6.4 The Added Risk Approach

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 with 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 the C_b and the MPA:

¹ Thus secondary poisoning may be assessed when deriving the SR_{ECO} for sediments, as shown by Van de Guchte et al. (2000).

² The HC_5 is the Hazardous Concentration for 5% of the species, as defined in Aldenberg and Jaworska 2000.

$$\text{MPC} = \text{Cb} + \text{MPA} \quad (30)$$

The MPA is calculated using a similar approach as the MPC for substances having no natural background concentration, see Sections 6.1, 6.2 and 6.3 (if secondary poisoning needs to be assessed, cf. Smit et al., 2000). 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 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 fulfill the need for micronutrients of species in the environment (Klepper et al., 1998).

The NC is defined as the background concentration (Cb) plus the Negligible Addition (NA):

$$\text{NC} = \text{Cb} + \text{NA}, \text{ where } \text{NA} = \text{MPA}/100. \quad (31)$$

The background concentration and the MPA are independently derived values.

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., 2000a). 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 deleterious, because of its contribution to biodiversity. Besides, at this 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., 2000a).

The added risk approach is in principle not used in deriving SRC_{ECO} values. This is based on the trigger value function, when the SRC_{ECO} determines the Intervention Value. Site-specific information on the background concentrations is required for establishing the (remediation) urgency. The added risk approach seems appropriate for deriving the SRC_{ECO} when background concentrations are not negligible compared to the SRC_{ECO} ¹.

6.5 Equilibrium Partitioning Method

The equilibrium partitioning method (EqP method) was originally proposed by Pavlou and Weston (1984) to develop sediment quality criteria for organic substances. Shea (1988) and DiToro et al. (1991) have described the concept in detail. Three assumptions are made when applying this method. First, it is assumed that bioavailability, bioaccumulation and toxicity are closely related to the pore water concentrations. Second, it is assumed that sensitivities of aquatic organisms are comparable with sensitivities of organisms living in the soil or sediment. Third, it is

¹ It is proposed to use the added risk approach when background concentrations are more than e.g. 25% of the SRC_{ECO} .

assumed that equilibrium exists between the chemical sorbed to the particulate sediment or soil organic carbon and the pore water, and that these concentrations are related by a partition coefficient (K_{oc}). For metals, empirical partition coefficients are used since the concentration of a metal in the pore water depends on other variables, in addition to the organic matter content, e.g. pH (Janssen et al., 1997).

The second assumption for the use of the EqP-method is based on the notion that many benthic organisms and terrestrial soft-bodied organisms such as earthworms and enchytraeids will be exposed mainly via the water or pore water. However, other species may take up substances from their food or directly from the soil or sediment, in which case there may be reasons not to adopt the EqP-method.

The Environmental Risk Limit for terrestrial and sediment species using the EqP-method is derived using the following equation:

$$ERL(sed / soil_{EP}) = ERL(water) * K_{p(ssoil / ssed)} \quad (32)$$

in which:

$ERL(sed/soil_{EP})$ = Environmental Risk Limit for terrestrial species using the EqP-method in mg/kg

$ERL(water)$ = Environmental Risk Limit for aquatic species in mg/l

$K_{p(ssoil/ssed)}$ = partition coefficient for standard soil or standard sediment in l/kg (cf. Section 3.3.2).

One of the current discussions on sediment water quality criteria is that the bioavailability of metals is highly affected in the sediment, e.g. by the Acid-Volatile Sulfide (AVS) content in relation with the Simultaneously Extracted Metals (SEM). If the ratio SEM/AVS is smaller than 1, the metals would not be bioavailable and would not cause any deleterious effects (Allen et al., 1993; DiToro et al., 1992; Swartz et al., 1985). For example, DiToro et al. (1990) showed that toxicity of cadmium to amphipods was not observed until the concentration of added cadmium to sediment exceeded that of sulphide. Later, DiToro et al. (1992) showed that the toxicity of cadmium and nickel to amphipods, oligochaetes and snails was not observed in spiked freshwater and marine sediments and contaminated sediments from a Superfund site. The latter two studies and others were used by Ankley et al. (1996) for a technical basis and proposal for deriving sediment quality criteria for metals. There thus seems to be many studies that indicate that the SEM/AVS concept may be used for evaluating site-specific toxicity of metals.

However, there are a number of comments on the SEM/AVS concept, which limits its use for a generic approach. Firstly, Ankley (1996) showed that in some cases there appeared to be a linear accumulation of metals with increasing sediment metal concentration irrespective of the SEM/AVS content. This questions the validity of the assumption that when the SEM/AVS < 1, the metals would not be bioavailable. Secondly, both the qualities of the SEM-data and the AVS-data are under recent discussion. The experimentally determined SEM values may underestimate the actual concentration of metals (Cooper and Morse, 1998), while the AVS values from pooled sediment samples may overestimate the actual AVS concentration in the top, aerobic sediment layer (Van den Berg et al., 1998).

Thirdly, relative to the SEM/AVS concentrations, sediment guidelines based upon dry weight-normalised concentrations were equally or slightly more accurate in predicting

both non-toxic and toxic results in laboratory tests (Long et al., 1998). These latter findings currently limit the value of the SEM/AVS ratio for risk assessment.

Fourthly, further research is required to the proposed SEM/AVS concept to better implement its significance (Ankley et al., 1996; Ankley, 1996; Mayer et al., 1996)

- for benthic organisms that have a habitat at or slightly above the sediment surface where aerobic conditions prevail, and the AVS-content will be very low;
- to protect aquatic systems from metal release associated with sediment suspension;
- for the transport of metals into the food web either from sediment ingestion or the ingestion of contaminated benthos; and
- for organisms that are capable of actively extracting substances from sediments, such as polychaetes, that may produce ligands for (essential) metals, to accelerate uptake.

Due to the several comments on the SEM/AVS concept, its use for a generic approach was not adopted. Instead, a modified equilibrium partitioning method is employed for metals (section 6.5.1).

6.5.1 The modified equilibrium partitioning method

For metals and metalloids in both sediment and soil, a modified EqP-method is applied. With this modification, MPCs are derived from those for water when insufficient toxicological data on sediment and soil organisms are available. It must be noted that originally the EqP-method normalises concentrations of organic substances in the solid phase to the organic carbon content (Pavlou and Weston, 1984). For metals and metalloids, the EqP-method was modified. The organic content normalisation was not applied but empirically derived sediment/water and soil/water partition or distribution coefficients were used for normalised standard soil or sediment (section 4.4.2.1).

We assume that the most important assumption for application of the modified EqP-method for metals and metalloids is a clear relationship between the concentration in water and the solid phase, for a range of concentrations even at low metal and metalloid levels. For a generic use, empirical soil/water ($K_{p,soil}$) are selected and sediment/water ($K_{p,sed}$) partition or distribution coefficients, which most realistically mimick distribution processes in the Dutch environment. The partition coefficients varied enormously, which is probably due to the different underlying physical-chemical processes that control the actual partitioning. The sources of the $K_{p,soil}$ and $K_{p,sed}$ values can be found in Crommentuijn et al. (1997a, 2000c).

6.6 Final harmonisation of ERLs

Harmonisation of ERLs is undertaken because substances in the environment distribute over the different environmental compartments, after initially being emitted into one or more of these compartments. For example, PAHs will be mainly emitted to air and water, via combustion sources, but will ultimately accumulate in soils, sediments, vegetation and biota. Due to these intercompartmental exchange processes, driven by fugacity or concentration gradients, harmonisation of the individual ERLs is needed.

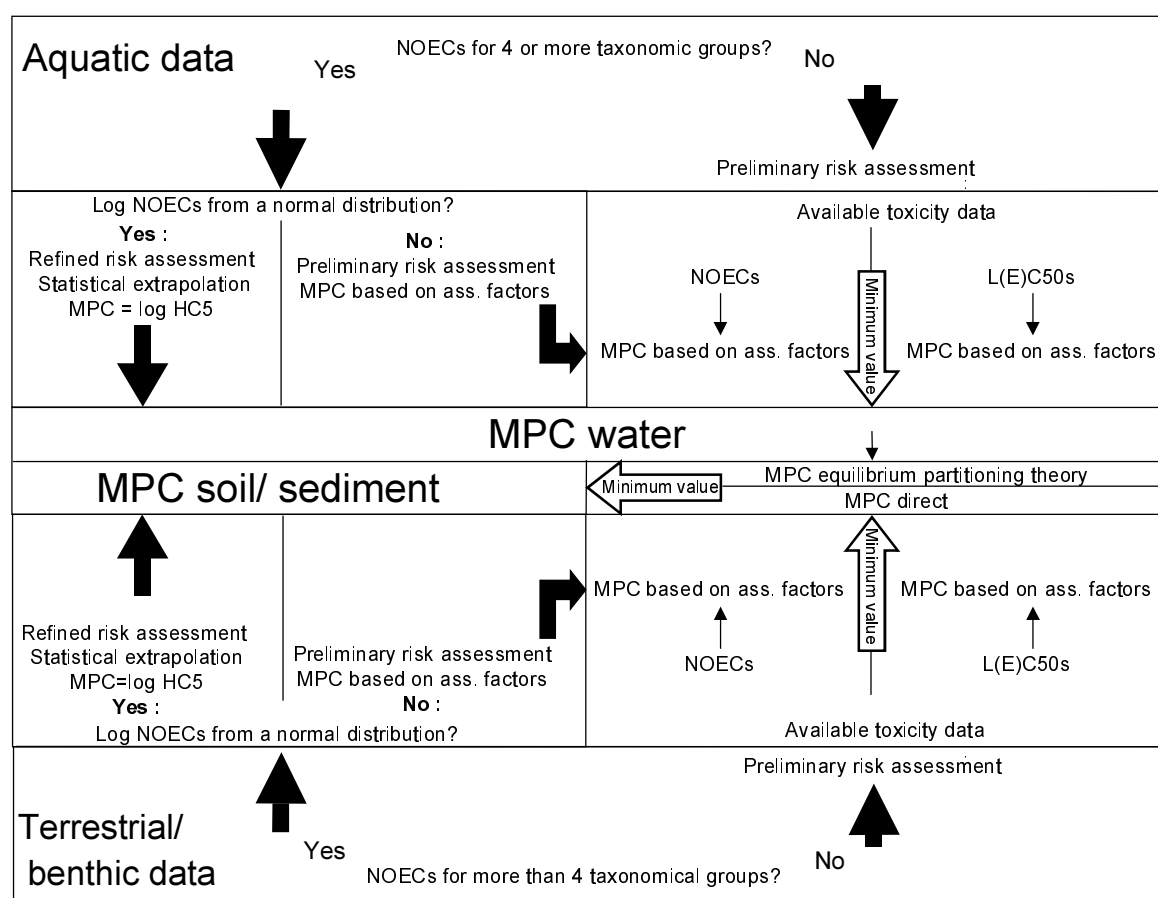


Figure 5: Diagram of the derivation and final harmonisation of the MPC. The 'minimum value rule (arrows)' only applies if the preliminary risk assessment for soil and or sediment is applied.

When independently derived ERLs for water, soil and sediment are available, ERLs for water, soil and sediment are harmonized (Figs. 5-6).

This is achieved by calculating the ERL for sediment or soil from the ERL for water, by applying the EqP-method (Section 6.5). The following guidelines are used to decide what determines the ERL:

- 1) If insufficient data for soil or sediment are available (e.g. no NOECs available), the ERL is derived from ecotoxicity data for water, using the EqP-method. If the MPC for surface water is based on a relatively large data set containing chronic data on several taxonomic groups while the ERL for soil or sediment is based on a limited data set, the ERL based on equilibrium partitioning may, on a case by case basis, be given more weight and be chosen as the MPC for soil or sediment.
- 2) If statistical extrapolation can be applied to terrestrial data, the MPC and $SRCECO$ are derived directly and no comparison with EqP-derived ERLs is made.
- 3) If condition 2 does not apply (i.e. no refined effects assessment) in principle the lowest value of the independently derived ERL for soil or sediment and the ERL resulting from the EqP method (eqn. 32) is taken as the harmonized ERL. This is done for the MPC as well as the $SRCECO$.

- 4) The ERLs for groundwater are set equal to the ERLs for surfacewater (freshwater), based on lack of evidence for differences in sensitivity (Notenboom et al., 2000).
- 5) The Negligible Concentration is calculated as MPC/100 for substances without a natural background, and is calculated as $(C_b + MPA/100)$ for substances with a natural background.
- 6) Independently derived ERLs can also be harmonized for human toxicological risk limits as discussed in Section 6.7.
- 7) ERLs derived for water are considered to be valid for dissolved concentrations. ERLs for total concentrations in water can be derived using EqP principles and (standardised) suspended matter content (Annex 10).

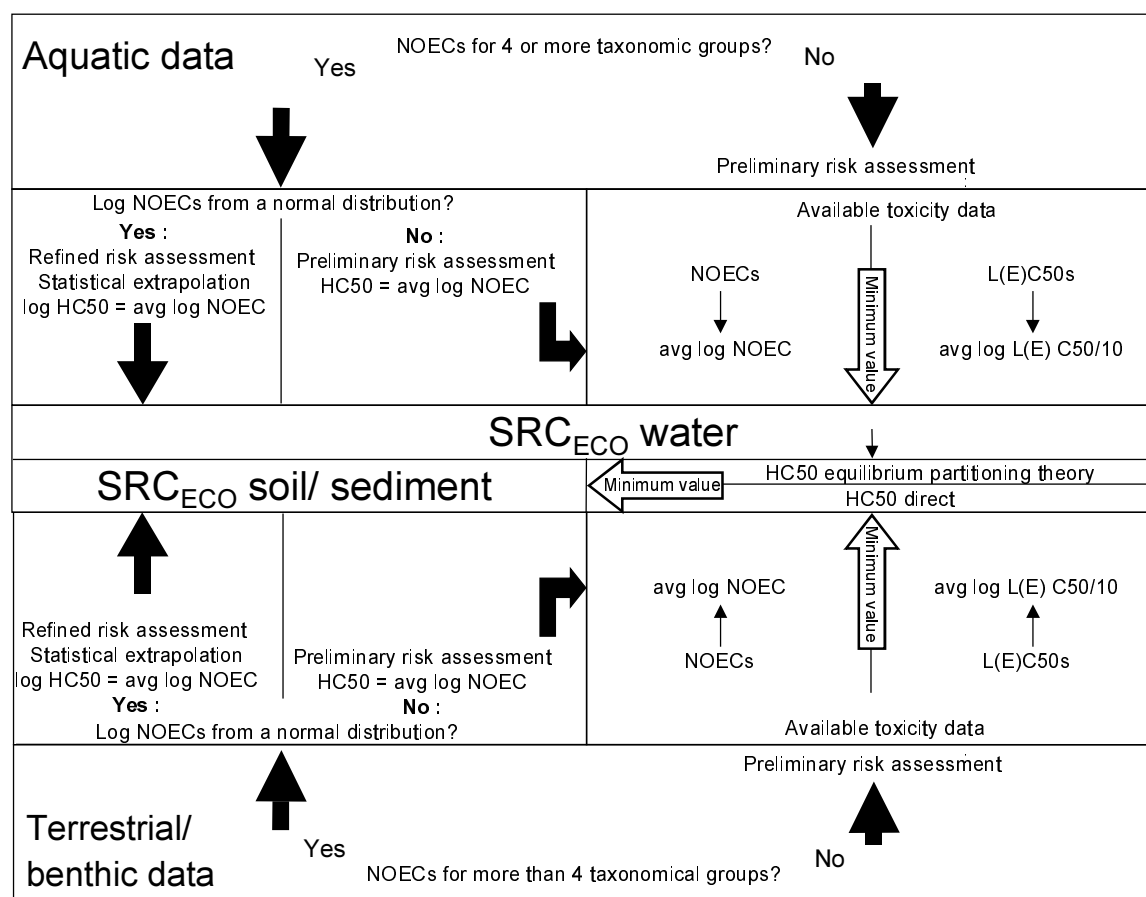


Figure 6: Diagram of the derivation and final harmonisation of the SRC_{ECO} . The 'minimum value rule (arrows)' only applies if the preliminary risk assessment for soil and or sediment is applied.

The final result is treated with caution and expert judgement may be needed. The uncertainties in both the ERLs and the partition coefficient are taken into account, such that unreliable ERLs (e.g due to unreliable K_p estimates or absence of sensitive species in a data set) are not preferred. The SRC_{ECO} for soil is always determined by the lowest ERL. In case of the MPC, deviations are possible based on expert judgement. Deviating assessment factors may be proposed for the derivation of ERLs if based on motivated expert judgement.

6.7 Human-Toxicological Risk Limits and integration with ERLs for air

Next to ERLs, Human Toxicological Risk Limits are derived in the Netherlands: the human-toxicological Maximum Permissible Risk (MPR). In the human-toxicological evaluation of chemical substances, generally a distinction is made between two standard approaches (Janssen and Speijers, 1997). The non-threshold approach is chosen for compounds that, on the basis of available evidence, are regarded as genotoxic carcinogens. In this case the MPR is defined as the exposure level with an excess lifetime cancer risk of 10^{-4} (VROM, 1989b). For other compounds a threshold approach is used. In that case the MPR is defined as an Acceptable Daily Intake (ADI) or Tolerable Daily Intake (TDI) (VROM, 1989b). This is explained in more detail in Annex 11. The Human-Toxicological Risk Limits are integrated with the ERLs in two different ways:

- 1) In the project 'Intervention values for soil clean-up and groundwater' the Intervention Value for soil clean up and groundwater is based on either the Human-Toxicological Serious Risk Concentration (SRC_{HUMAN}) or the Ecotoxicological Serious Risk Concentration (SRC_{ECO}) (Figure 1). The SRC_{HUMAN} and the SRC_{ECO} are expressed as a concentration in the soil and are distinctly derived values (Swartjes, 1999). The SRC_{HUMAN} is based on the MPR. The MPR is converted into a concentration in the soil using the model C-soil (Van den Berg and Roels, 1991; Van den Berg, 1994). In principle the lower of the two, the SRC_{HUMAN} or the SRC_{ECO} , is chosen as proposed for the Intervention Value.
- 2) In the project 'Setting Integrated Environmental Quality Standards' all MPCs and NCs are harmonised for the different environmental compartments: water, sediment and soil. For volatile substances, MPCs and NCs have also been harmonised with Human-Toxicological Risk Limits (Van de Plassche and Bockting, 1993). This procedure is described in Annex 11. For these volatile substances it is assumed that inhalation through air is the predominant route of exposure for man. Harmonisation of the Human-Toxicological Risk Limits for air with those for soil and water is done using the multimedia fate model SimpleBox (Van de Meent, 1993). On the basis of the MPC for soil and water the resulting equilibrium concentration in air is calculated and compared with the Human-Toxicological Risk Limit for air. In principle the MPC for water and soil has to be adjusted if the corresponding equilibrium concentration in air exceeds the Human-Toxicological Risk Limit (Van de Plassche and Bockting, 1993; Mennes et al., 1998). However, the uncertainties in the MPCs, in the Human-Toxicological Risk Limits and in the input parameters of the model are taken into account. Harmonisation of MPCs for water, sediment and soil with Human-Toxicological Risk Limits based on multi-route exposure patterns, is the subject of continuing study (Mennes et al., 1995; Mennes et al., 1998 cf. section 7.2.3.).

7. Concluding remarks

7.1 Current ERLs and EQSs

In the last decade, the National Institute of Public Health and the Environment has derived ERLs for approximately 200 substances, that belong to several chemical classes, such as metals, PAHs, organic substances, pesticides, etc. The Dutch government has used most of them to set EQSs. For some of the recently derived ERLs, EQSs have not yet been set. For some other ERLs such as PCBs (Annex 7), the government has asked for additional, independent advice from the Dutch National Health Council and the Dutch Technical Soil Protection Committee on the methodology that is used to derive ERLs. The ERLs can be found in RIVM reports or in the literature; the EQSs can be found in IWINS (1997) and VROM (2000) or below (Table 23).

Table 23. References to numerical values of the Environmental Risk Limits (ERLs) and Environmental Quality Standards (EQSs) in The Netherlands.

MPCs and NCs	
<ul style="list-style-type: none"> Chlorophenols Several volatile compounds Substances with a potential for secondary poisoning Polycyclic aromatic hydrocarbons^a Pesticides 	Crommentuijn et al. (2000b) ^a A more extensive publication on deriving ERLs for PAHs can be found in Kalf et al. (1997).
<ul style="list-style-type: none"> (Trace) metals and a metalloid 	Crommentuijn et al. (2000c) Smit et al. (2000)
<ul style="list-style-type: none"> Anilines 	Reuther et al. (1998)
<ul style="list-style-type: none"> Polychlorinated biphenyls 	Van Wezel et al. (2000a)
<ul style="list-style-type: none"> A series of trace metals and an organosilicon substance 	Van de Plassche et al. (1999)
<ul style="list-style-type: none"> Phthalates 	Van Wezel et al. (2000b)
<ul style="list-style-type: none"> Rare earth elements 	Sneller et al. (2000)
SRC_{ECO}	
<ul style="list-style-type: none"> Metals Inorganic contaminants Aromatic contaminants PAHs Chlorinated hydrocarbons Pesticides Other pollutants 	Swartjes (1999)
EQSs	
MPCs and Target Values For different substances with ERLs before 1997	Crommentuijn et al. (2000b); Crommentuijn et al. (2000c)
Intervention Values and Target Values for different substances with SRC _{ECO} before 2000	VROM (2000)

An evaluation of the MPCs that were derived before 1998 shows that for organic substances and pesticides, 15 % of the MPCs were derived using the Refined effect assessment method, 30% was derived using Preliminary effect assessment, and 55% was derived following the EqP-method (Table 24). For metals, 31% of the MPCs were derived using the refined effect assessment method, 19% was derived using the preliminary effect assessment, and 50% was derived using the (modified) EqP-method (Table 24). It is expected that the uncertainty of the MPCs generally increases in the following order: refined effect assessment < preliminary effect assessment < the EqP-method. This order is purely based on the number of available ecotoxicity studies. Chapman et al. (1998) grossly corroborate this relative order in uncertainties. Many of the ERLs may thus be better based if more ecotoxicological data were available. Given these uncertainties and new scientific developments, the Dutch government re-evaluates the EQSs every 5 years, if needed, or at shorter time intervals if there is sufficient scientific reason to do so (IWINS, 1997).

Table 24. Evaluation of the underlying basis for the MPCs that were derived before 1997 by the National Institute of Public Health and the Environment (RIVM) and served to set EQSs by the Dutch government (Crommentuijn et al., 2000b; Crommentuijn et al., 2000c).

Method	Water	Soil	Sediment	Percentage of total
<i>Organic substances and pesticides (n=150)</i>				
Refined effect assessment	67	0	0	15%
Preliminary effect assessment	85	49	0	30%
EqP-method	0	100	148	55%
<i>Metals (n=18)</i>				
Refined effect assessment	12	5	0	31%
Preliminary effect assessment	6	4	0	19%
EqP-method	0	9	18	50%

7.2 Perspective

7.2.1 Statistical Issues

ERLs as defined in this guidance document have been derived using state-of-the-art methods where possible, but uncertainty remains. Some of these uncertainties are simply caused by too little information on the ecotoxicity of a given substance. Other uncertainties are due to inherent methodological uncertainty, i.e. there is no single conclusive approach. Statistical methods in deriving ERLs are being refined continuously (e.g. Aldenberg and Jaworska, 2000; Posthuma et al., 2001) and new developments will be screened for use in deriving ERLs. A recent review of the use of refined risk assessment for deriving ERLs suggests that the available data should be analysed more thoroughly before deriving ERLs (Suter et al., 2001). Statistical issues such as alternative distributions, the goodness of fit, the presence of poly-modality due to a specific mode of action or taxonomic differences will be studied in the near future.

Probabilistic modeling is currently receiving serious attention (Slob and Krajnc 1994, Van Wezel et al., 2000; Traas et al., 2001) and can become a logical extension of

refined effect assessment where ERLs are now report with their confidence limits. In these type of models, all relevant parameters that are used to calculate ERLs such as sorption coefficients, bioconcentration factors and acute-chronic ratios (ACRs) are characterised by distributions (Appendix 7). These distributions are based on prior information that is available from experiments, databases or experience. The promise of such models is that by using all available information instead of median or worst case estimates of parameters, the uncertainty of the ERLs is quantified and decisions can be based on the confidence limits of the ERLs and the required safety margin. At the moment, routine application of probabilistic risk assessment is hampered by data limitations.

7.2.2 Bioavailability

ERLs are derived for generic purposes, and therefore, for site-specific risk assessment, site-specific conditions need to be taken into account. For example, bioavailability and partitioning of substances in the field may be different from that in laboratory tests and may thus result in mis-interpretation of the risk of concentrations found in the field.

For compounds in water where speciation depends on pH, recalculation of toxicity to the relevant species (of the compound) and normalisation to a specific pH (range) may be needed. Recalculations using Henderson/Hasselbalch concentrations (cf. van Wezel, 1998) can be considered.

Recent findings for the bioavailability of metals in soil to soil invertebrates indicate a distinction between soft- and hard bodied invertebrates (Peijnenburg et al., 2001). Bioavailability will be studied in more detail in the near future in order to understand the physico-chemical and the biological aspects of bio-availability and their interaction. Essential metals need special attention since organisms can influence the bioavailability of toxicants. This should allow the refinement of models for partitioning, bioaccumulation and toxicity based on critical tissue concentrations. These models could then be used with the current toxicity data for developing ERLs that are corrected for bioavailability.

7.2.3 Integration of human risk limits

The present guidance for deriving ERLs is mainly based on ecotoxicological risks. As indicated in section 6.8, human risk is integrated in the derivation of the SRC, but is not routinely incorporated in the derivation of the MPC. Since the MPC is meant to provide protection for both humans and the ecosystem, this matter requires additional attention in the near future.

7.2.4 Data limitations

Despite the large efforts in environmental chemistry and ecotoxicology over the last decades there is still a huge lack of data. A way to overcome data limitations is to use QSARs to estimate toxicity for organisms and use this as input in the methods to derive ERLs. Additional work is in progress to update the QSARs that are currently in use. Since QSAR estimates are uncertain, their use as input in statistical extrapolation methods may require additional attention (cf. Appendix 8). Analysis of toxicity data bases may yield more reliable estimates for extrapolation or assessment factors when based on related compounds with a similar mode of action (De Zwart, in prep.) and will be considered for inclusion in guidance. The present guidance reflects the current

use of available data and methods to derive ERLs but experience has shown that the methods are being revised and refined in a continuous process. This guidance document only reflects the current procedure and much can be learned from new developments, comments and critical evaluation of the present procedure.

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Annex 1A. Taxonomic position of selected groups of aquatic species

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

Annex 1B: Taxonomic position of selected groups of soil species

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

Annex 2. Literature search profiles

A Literature search profile for soil organisms and macrophytes

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

B Literature search profile for aquatic organisms

f bc=(13000 or 13100 or 13300 or 13500 or 13700 or 13900 or 14100)"
 f bc=(14300 or 14700 or 35100 or 35200 or 35000 or 39000 or 41000)"
 f bc=(45000 or 45300 or 51600 or 51000 or 61000 or 61200 or 61500)"
 f bc=(65000 or 65500 or 75100 or 75102 or 75108 or 75110 or 75112)"
 f bc=(75114 or 83000 or 83100 or 83300 or 83400 or 83500 or 85200)"
 f bc=(85206 or 25340 or 25395 or 75314 or 75342 or 75318 or 75300)"
 f bc=(75338 or 85300 or 85304 or 85306 or 61600 or 65200)"
 f water boatman or waterboatman or photobacterium or pseudomonas"
 f 1 to 8"
 f 9 not (drosophila or fruit fly or fruit flies)"
 f sc=(07502 or 07510 or 07512 or 07514 or 22501 or 22506 or 37015)"
 f sc=(07506 or 07516)"
 f 11 or 12"
 f 10 and 13"
 f water# or freshwater# or fresh water# or pond# or lake# or river# or sea"
 f seas or ocean? or estuar? or saltwater# or salt water# or brackish or marine"
 f saline or brine or seawater or tidal or coast? or (aquatic or salinity)/ti"
 f 15 to 17"
 f 14 and 18"
 f (reproduct? or inhibit? or impact or hazard? or risk# or suppression)/ti"
 f (influence# or response# or susceptibilit? or interaction# or effect or effects)/ti"
 f (mortalit? or lethal? or survival or growth or tolerance or sensitivit? or intoxication)/ti"
 f ec50 or lc50 or noec or matc or pnec or pec or treshhold limit or ld50"
 f (toxic? or ecotoxic?)/(ti;ut)"
 f 20 to 24"
 f 19 and 25"

f 26 not la=(ru or ch or cz or it or po or sp or ja or hu or bu)"

C Literature search profile for birds

f bc=(85500 or 85504 or 85506 or 85514 or 85518 or 85520 or 85522 or 85524 or 85526)"

f bc=(85534 or 85536 or 85548 or 85550 or 85554 or 85556 or 85564)"

f 1 to 2"

f sc=(22501 or 22506 or 37015 or 54600)"

f 3 and 4"

f 5 not la=(ch or ja or po or bu pr hu or ru or it or sp or cz)"

D Literature search profile for mammals

Search using the database TOXLINE:

f (rat or rats or mice or mouse or dog or dogs or cat or cats or pig or pigs)/(ti;ct)"

f (hamster# or guinea pig# or mammal? or monkey#)/(ti;ct)"

f 1 to 2"

f (reproduct? or inhibit? or impact or hazard? or risk# or suppression)/ti"

f (influence# or response# or susceptibilit? or interaction# or effect or effects)/ti"

f (mortalit? or lethal? or survival or growth or tolerance or sensitivit? or intoxication)/ti"

f ec50 or lc50 or noec or matc or pnec or pec or treshold limit or ld50"

f (toxic? or ecotoxic?)/(ti;ct)"

f 4 to 8"

f 3 and 9"

f 10 not la=(polh or bulg or japn or chin or span or czech or ital)"

E Literature search profile for partition coefficients

For biosis via the host DIMDI:

f (sorption or adsorption or partitioning or cosolven? or partition)/ti"

f (langmuir or freundlich or sorptive or batch experiment)/ti"

f (equilibri? or isotherm or koc or kd or kp)/ti"

f 1 to 3"

f (soil or soils or sediment? or soil water system? or organic matter or organic carbon)/ti"

f 4 and 5"

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

For chemical abstracts via the host DIALOG:

s sorption or adsorption or desorption or partitioning or cosolven? or partition"

s complexation or langmuir or freundlich or sorptive or bioavailability"

s complex(w)formation or fractionation or precipitation or coprecipitation"

s remobili!ation or equilibri? or partition or isotherm or interaction? or koc or kd or kp"

s S1 or S2 or S3 or S4

s liquid(w)solid or suspended(w)matter or sediment? or suspended(w)particles"

s sludge or soil? or particulate(w)matter or solid(w)phase or liquid(w)phase"

s suspended(w)solid? or suspended(w)material? or interstitial(w)water"

s porewater or groundwater or dissolved(w)matter or dissolved(w)phase"

s third(w)phase or suspended(w)sediment or colloid? or aquifer"

s S6 or S7 or S8 or S9 or S10

s S5 and S11

Annex 3A. Aquatic toxicity data tables

Table A3-1: Aquatic species, chronic toxicity example table

Species	Species Prop.	Anal.	Test Type	Subst. Purity	Test Water	pH	Hardness	Exp Time	Criterion	Test Endpoint	Value (mg/l)	Notes	Rreference
algae													
Chlorella emersoni		N	-	-	-	-	-	7 d	NOEC	Growth	2.8		Melin & Egneus, 1983
Pseudokirchneriella subcapitata		Y	S	-	-	-	-	10 d	NOEC	Growth	0.21		Adams et al., 1995
Pseudokirchneriella subcapitata		N	-	-	-	-	-	7 d	NOEC	Growth	2.8		Melin & Egneus, 1983
Scenedesmus subspicatus		Y	-	-	-	-	-	7 d	NOEC	Growth	6.1		Hüls AG, 1991
crustacea													
Daphnia magna		N	CF	99.5	-	7.9	85	16 d	NOEC	Repro	0.56	1	McCarthy & Whitmore, 1985

1: fecundity

Table A3-2: Aquatic species, acute toxicity example table

Species	Species Prop.	Anal.	Test Type	Subst. Purity	Test Water	pH	Hardness	Exp. Time	Criterion	Endpoint	Value (mg/l)	Notes	Reference
protozoa													
Tetrahymena pyriformis		N	S	-	-	-	-	48 h	EC50	Growth	7.0		Staples et al., 1997 (review)
algae													
Pseudokirchneriella subspicata		Y	S	-	-	7.8	25-50	96 h	EC50	Growth	0.40		Adams et al., 1995
Scenedesmus subspicatus		N	S	-	am	8.0	-	48 h	EC50	Growth	3.5	1	Kühn & Pattard, 1990
crustacea													
Daphnia magna		N	S	99.5%	-	-	85	48 h	LC50	Mort	5.2		McCarthy & Whitmore, 1985
Gammarus pseudolimnaeus		N	CF	-	-	-	-	96 h	LC50	Mort	2.1		Mayer & Sanders, 1973
Insecta													
Chironomus plumosus	3 rd instar	Y	S	-	nw	7.4	270	48 h	EC50	Immo	0.76		Streufert et al., 1980
Paratanytarsus parthenogenica		Y	S	-	-	7.8	25-50	96 h	LC50	Mort	6.3		Adams et al., 1995
Pisces													
Lepomis macrochirus	1.4 g	N	S	100%	-	7.1	44	96 h	LC50	Mort	0.73		Mayer & Eilersieck, 1986
Perca flavescens	0.8 g	N	CF	100%	-	7.6	314	96 h	LC50	Mort	0.35		Mayer & Eilersieck, 1986

1: biomass

Annex 3B. Soil toxicity data tables

Table A3-3: Soil species, chronic toxicity, example table

Species	Species properties (age, sex)	Soil type	pH	o.m. [%]	Clay [%]	Temp [°C]	Exp. time	Criterion	Test Endpoint	Result test soil [mg/kg dw]	NOEC stand. soil [mg/kg dw]	Notes	Reference
Bacteriophyta													
Actinomycetes		alluvial	6.6	0.31	-	27	10d	EC15	growth	80	200	1	Bakalivanov & Kostov, 1981
Actinomycetes		-	5.7	2.75	-	27	10d	EC17	growth	80	145	2	Bakalivanov & Kostov, 1981
denitrifiers		-	6.6	2.1	17	25	6h	EC20	growth rate	100	238	3	Pell et al., 1998
Insecta													
Folsomia candida	10-12 days	sandy loam	-	10	20	-	28d	NOEC	Repro	170	170	4	Jancke, 1989
Folsomia candida	10-12 days	sandy loam	-	10	20	-	28d	EC10	Repro	140	140	5	Jancke, 1989

- 1: purity unknown; one conc tested (80 mg/kg); NOEC growth inhibition as EC15/2, based on o.m. content of 2%
2: purity unknown; one conc tested (80 mg/kg); NOEC growth inhibition as EC17/2
3: one concentration tested (100 mg/kg); NOEC on growth rate as EC20/2
4: Hatching, 43% effect at lowest concentration, NOEC as EC43/3
5: NOEC egg production as EC10, graphical extrapolation

Table A3-4: Soil, microbial processes and enzyme activity, example table

Process/Activity	Soil type	pH	o.m. [%]	Clay [%]	Temp [°C]	Exp. time [h]	Criterion	Result test soil [mg/kg dw]	NOEC stand soil [mg/kg dw]	Test Endpoint	Notes	Reference
Microbial processes												
basal respiration	loam	6.5	12	18	22	3d	NOEC	20	17	increase CO ₂	1	Wardle & Parkinson, 1990
Substrate Induced Respiration	loam	6.5	12	18	22	3d	NOEC	20	17	increase CO ₂	2	Wardle & Parkinson, 1990
Denitrification	-	6.6	2.1	17	25	2h	EC12	100	238	stimulation	3	Pell et al., 1998
Ammonification	-	6.6	2.1	17	25	6h	EC9	100	476		4	Pell et al., 1998
Enzymatic activity												
Phosphatase	organic	7.2	46	-	28	2h	EC46	5	0.56		5	Tu, 1981
Urease	silt loam	5.4	3.7	20	22	70d	NOEC	0.1	0.27		6	Lethbridge et al., 1981

- 1: purity unknown
2: purity unknown; glucose as substrate
3: one concentration tested; NOEC=LOEC/2
4: one concentration tested; NOEC=LOEC
5: purity >94%, NOEC as EC53/3 based on o.m. content of 30%
6: data from Dennenman & Van Gestel, 1990

Annex 3C. equilibrium partition coefficient data table

Table A3-5 : Equilibrium partition coefficients, example table

Test substance	Purity	Soil Type	% OC	pH	CEC mmol/kg	Solid/water g/l	Mass balance	Equil. time	logKoc	Notes	Reference
Substance A		sandy till	0.0588	4.7	91	200	N	72 h	2.69		Lokke (1984)
		melt water sand	0.0529	6.1	14	200	N	72 h	2.55		Lokke (1984)
		clayey till	0.1294	7.6	405	200	N	72 h	2.26		Lokke (1984)
Substance B		silt loam	1.49	5.0	-	200	Y	18 h	1.47		Walton et al. (1992)
		sandy loam	0.66	4.4	-	200	Y	18 h	1.26		
Substance C		sediment	0.85	-	-	125-875	N	6 h	0.70-1.08	1	Zhao & Lang (1996)
									1.04-1.14	2	
									3.91	3	Bokting et al. (1993)
		-	-	-	-	-	-	-	4.78	4	Bockting et al. (1993)

- 1: observed partition coefficient at different solid concentrations
- 2: true partition coefficient at different solid concentration, corrected for dissolved organic carbon and nonsettling micro-particles
- 3: Gerstl (1990)
- 4: Di Toro (1991)

Annex 3D. Bioconcentration factors data table

Table A3-6: Whole body bio-concentration factors (BCFs) for fish, example table

Species	Species properties	Test Type	Subst Purity(%)	Test Water	pH	Salinity [g/l]	Exp. time [d]	Exp. Concn.	Time to Equilibrium	dw/ww ratio [g dw/gww]	BCF [l/kg ww]	Notes	Reference
Cyprinodon variegatus		CF	99.9	ns	-	17.4	28d	1.3, 3.3	-		9,400	1	Parrish et al., 1976
Cyprinodon variegatus		CF	100	ns	-	17.2	189	0.5, 0.8, 1.7	-		14,000	1	Parrish et al., 1978
Cyprinodon variegatus		CF	100	ns	-	17.5	28	0.5, 0.8	-		20,000	2	Parrish et al., 1978
Cyprinodon variegatus		CF	100	ns	-	17.2	28	0.5, 0.8	-		9,000	3	Parrish et al., 1978

- 1: eggs produced in the laboratory by adults collected from a natural population; BCF's determined at end of exposure
- 2: F1 juveniles, from first spawn of parents (from eggs: see 1), exposed to the same conc's
- 3: as for note 2), from second spawn

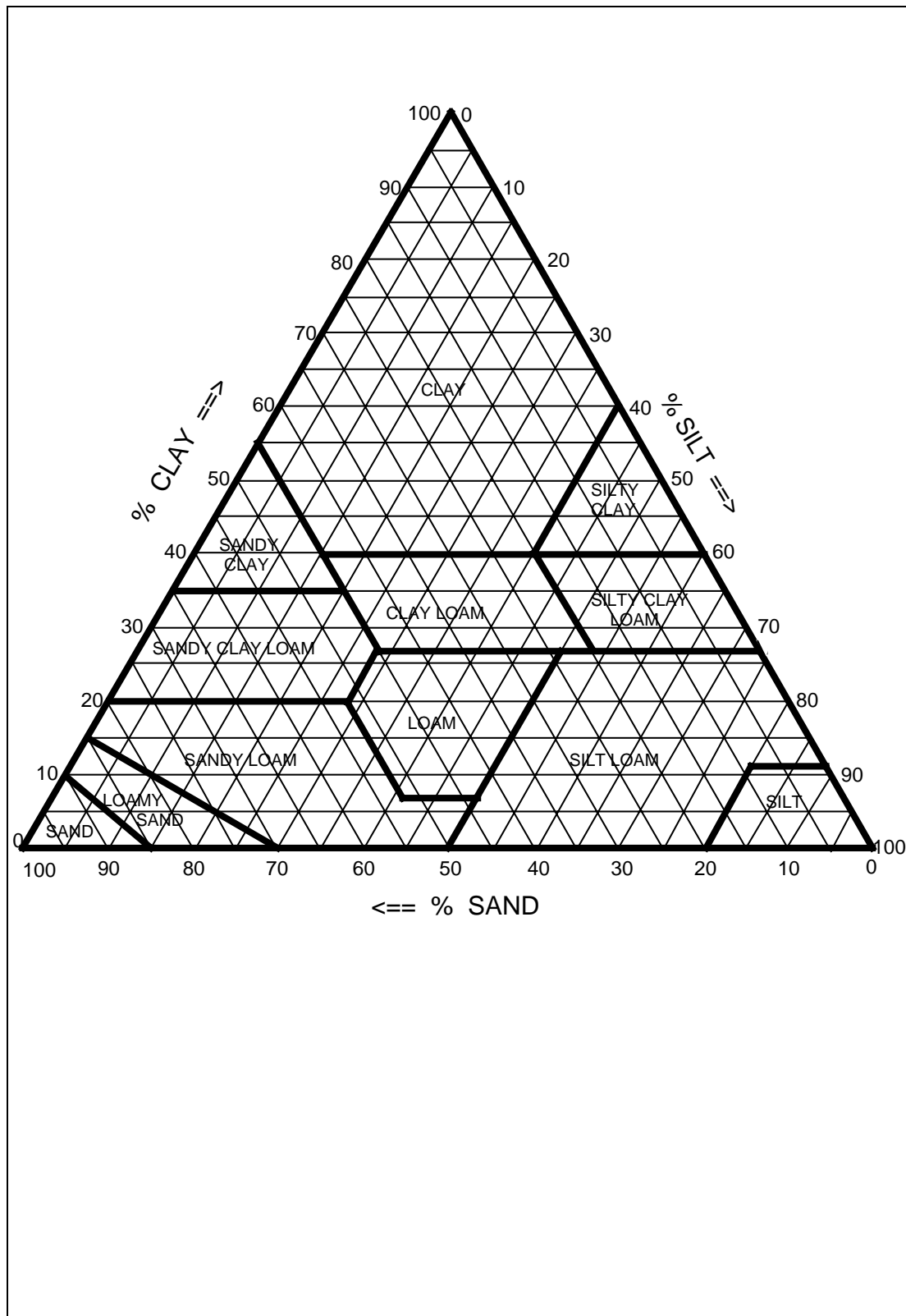
Annex 3E. bird and mammal toxicity data table

Table A3-7: bird and mammal toxicity data, example table

Species	Species properties (age, sex)	Substance Purity	Application route	Exposure Time	Criterion	Test Endpoint	Effect Conc'n Gavage mg/(kg bw.d)	Effect Conc'n Diet mg/kg diet	Notes	Reference
Birds										
Anas platyrhynchos	4-5 m (f)		oral	acute	LD50	Mort	1200	4800	1	Hudson, Tucker & Haegele (19xx)
Callipepla californica	10 d	72%	diet	5d	LC50	Mort		858	2	Hill & Heath (1975)
	12 m (m)		oral	acute	LD50	Mort	14.1	28.2	3	Hudson, Tucker & Haegele (19xx)
Colinus virginianus		72%	diet	5d	LC50	Mort		331	4	Agrochemical Handbook (1987)
Mammals										
Mouse	(m,f)		oral		LD50	Mort	0.38-1.50	3.2-12.5	5	Hayes & Laws, 1991
Dog	(f)		oral		LD50	Mort	4640	185600	6	IPCS/EHC draft, 1992

- 1. Recalculated using a conversion factor of 4 (kg bw.d/kg food) (cf. Table 11).
- 2. Slope parameter 3.796 from probit fit on log concentration.
- 3. Recalculated using a conversion factor of 2 (kg bw.d/kg food) (cf. Table 11).
- 4. Slope parameter 4.866 from probit fit on log concentration.
- 5: In Oil. Recalculated using a conversion factor of 8.3 (kg bw.d/kg food) (cf. Table 11).
- 6: Recalculated using a conversion factor of 40 (kg bw.d/kg food) (cf. Table 11).

Annex 4. American soil classification system



Annex 5. Glossary

BCF	BioConcentration Factor: the ratio of the test substance concentration in (part of) an organism (e.g. fish, daphnid, plant) to the concentration in a medium (e.g. water, soil) at steady state.
BSAF	Biota-Sediment Accumulation Factor: the ratio of the test substance concentration in an organism (e.g. insect larvae, or fish) to the concentration in the sediment at steady state. The organism can be exposed by water and food exposure routes.
BmB	Abbreviation in Dutch for “Besluit Milieutoelatingseisen Bestrijdingsmiddelen”.
Cb	Background Concentration
CSR	Centrum voor Stoffen en Risicobeoordeling (Dutch), Centre for Substances and Risk Assessment (English)
CTB	College voor de Toelating van Bestrijdingsmiddelen (Dutch), Board for the Authorisation of Pesticides (English).
DGM	Directoraat-Generaal Milieubeheer (Dutch); Directorate General for Environmental Protection (English)
DT50	Time in which 50% of the parent compound has disappeared from soil or water by transformation or degradation (under standard conditions). See degradation and transformation
EC50	Median Effective Concentration: 1. the concentration resulting in a 50% change in a parameter (e.g. algal growth) relative to the control 2. the concentration at which a particular effect (e.g. daphnia immobilization) is observed in 50% of the organism population relative to the control
ERL	Environmental Risk Limits serve as advisory values to set environmental quality standards (EQS) by the government for various policy purposes.
EU	European Union
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice: a set of rules describing how a laboratory should work, how it should be organised and how it can produce valid data; GLP principles are described by e.g. OECD
H	Henry’s law air-water partition coefficient; the ratio between the partial pressure in the gas phase of a compound and its concentration in water. Henry’s law constant can be used with units ($\text{Pa}\cdot\text{m}^3\cdot\text{mol}^{-1}$, synonym is H') or unitless (synonym is H)
HC5	Hazardous Concentration for 5% of the species, a 5 th percentile value (concentration) derived from species sensitivity distributions. This concentration is expected to be protective of the whole ecosystem.
I-Value	Intervention value. This is an environmental quality standard (EQS) of the Dutch government used for various policy purposes. It can be derived for soil, sediment or groundwater and is based on serious risks for man or the ecosystem.
IC50	median Inhibitory Concentration: the concentration resulting in a 50% inhibition of growth relative to the control
INS	Abbreviation in Dutch for the project ‘Setting of Environmental Quality Standards’
IWINS	Abbreviation in Dutch for ‘Interdepartementale Werkgroep Integrale Normstelling Stoffen’, now Stuurgroep INS.
K_{aw}	air-water partition coefficient. See Henry’s law constant

K_f	Freundlich coefficient: a soil-water partition coefficient —or sorption coefficient— dependent on the exponent $1/n$ (n is an empirical entity which describes the non-linearity of an adsorption isotherm)
K_{oc}	sorption coefficient normalised to the fraction of organic carbon in soil
K_{om}	sorption coefficient normalised to the fraction of organic matter in soil
K_{ow}	octanol-water partition coefficient
K_s/l	soil-water partition coefficient independent on the ratio $1/n$ (n is an empirical entity which describes the non-linearity of an adsorption isotherm)
LC50	median Lethal Concentration: a statistically derived concentration that can be expected to cause death in 50% of animals exposed for a specified time
LD50	median Lethal Dose: statistically derived single dose that can be expected to cause death in 50% of dosed animals
LNv	Ministerie van Landbouw, Natuurbeheer en Visserij (Dutch), Ministry of Agriculture, Nature Management and Fisheries
MJP-G	Abbreviation in Dutch for ‘Multi-year crop protection plan’
MPA	Maximum Permissible Addition
MPC	Maximum Permissible Concentration
NC	Negligable Risk Concentration
NOEC	No-Observed-Effect-Concentration: the highest observed concentration without adverse effects
OC	organic carbon
OM	organic matter
P	vapour pressure
PAF	Potentially Affected Fraction, the probability that a species randomly drawn from an ecosystem is exposed (at a given concentration) above its NOEC.
PARTITION COEFFICIENT	Ratio of the distribution of a substance between two phases when the heterogeneous system (of two phases) is in equilibrium; the ratio of concentrations (or, strictly speaking, activities) of the same molecular species in the two phases is constant at constant temperature
PNEC	Predicted No Effect Concentration
RIVM	Abbreviation in Dutch for the National Institute of Public Health and Environmental Protection
RIZA	Abbreviation in Dutch for the National Institute of Inland Water Management.
S	Water solubility
SGB	Abbreviation in Dutch for Steering Group Pesticide Policy “Stuurgroep Bestrijdingsmiddelenbeleid”
SRC	Serious Risk Concentration, based on either ecotoxicological data (SRC_{ECO}) or human toxicological data (SRC_{HUMAN})
SAS	Abbreviation in Dutch for Directorate Chemicals, Waste and Radiation Protection
TCB	Technical Soil Protection Committee, and advisory council of the Dutch Government,
TGD	Technical Guidance Documents
VROM	Abbreviation in Dutch for the Ministry of Housing, Spatial Planning and the Environment

Annex 6. Extrapolation factors for estimating log hazardous concentrations.

HC5 Extrapolation Constants Table acc. to Aldenberg and Jaworska (2000).
For deriving the MPC, the median HC5 extrapolation constant is used

n	lower	median	upper	n	lower	median	upper
2	26.25968	2.33873	0.47479	51	2.06007	1.65473	1.33216
3	7.65590	1.93842	0.63914	52	2.05532	1.65453	1.33486
4	5.14388	1.82951	0.74330	53	2.05071	1.65435	1.33749
5	4.20268	1.77928	0.81778	54	2.04625	1.65417	1.34005
6	3.70768	1.75046	0.87477	55	2.04193	1.65399	1.34254
7	3.39947	1.73179	0.92037	56	2.03774	1.65383	1.34497
8	3.18729	1.71872	0.95803	57	2.03367	1.65366	1.34734
9	3.03124	1.70906	0.98987	58	2.02972	1.65351	1.34965
10	2.91096	1.70163	1.01730	59	2.02589	1.65336	1.35191
11	2.81499	1.69574	1.04127	60	2.02216	1.65321	1.35412
12	2.73634	1.69096	1.06247	61	2.01853	1.65307	1.35627
13	2.67050	1.68700	1.08141	62	2.01501	1.65294	1.35837
14	2.61443	1.68366	1.09848	63	2.01157	1.65281	1.36043
15	2.56600	1.68082	1.11397	64	2.00823	1.65268	1.36244
16	2.52366	1.67836	1.12812	65	2.00498	1.65256	1.36441
17	2.48626	1.67621	1.14112	66	2.00180	1.65244	1.36633
18	2.45295	1.67433	1.15311	67	1.99871	1.65232	1.36822
19	2.42304	1.67266	1.16423	68	1.99569	1.65221	1.37006
20	2.39600	1.67116	1.17458	69	1.99274	1.65210	1.37187
21	2.37142	1.66982	1.18425	70	1.98987	1.65199	1.37364
22	2.34896	1.66861	1.19330	71	1.98706	1.65189	1.37538
23	2.32832	1.66752	1.20181	72	1.98431	1.65179	1.37708
24	2.30929	1.66651	1.20982	73	1.98163	1.65170	1.37875
25	2.29167	1.66560	1.21739	74	1.97901	1.65160	1.38038
26	2.27530	1.66475	1.22455	75	1.97645	1.65151	1.38199
27	2.26005	1.66398	1.23135	76	1.97394	1.65142	1.38357
28	2.24578	1.66326	1.23780	77	1.97149	1.65133	1.38511
29	2.23241	1.66259	1.24395	78	1.96909	1.65125	1.38663
30	2.21984	1.66197	1.24981	79	1.96674	1.65117	1.38812
31	2.20800	1.66140	1.25540	80	1.96444	1.65109	1.38959
32	2.19682	1.66086	1.26075	81	1.96218	1.65101	1.39103
33	2.18625	1.66035	1.26588	82	1.95997	1.65093	1.39244
34	2.17623	1.65988	1.27079	83	1.95781	1.65086	1.39383
35	2.16672	1.65943	1.27551	84	1.95568	1.65078	1.39520
36	2.15768	1.65901	1.28004	85	1.95360	1.65071	1.39654
37	2.14906	1.65861	1.28441	86	1.95156	1.65064	1.39786
38	2.14085	1.65823	1.28861	87	1.94955	1.65058	1.39916
39	2.13300	1.65788	1.29266	88	1.94759	1.65051	1.40044
40	2.12549	1.65754	1.29657	89	1.94566	1.65045	1.40170
41	2.11831	1.65722	1.30035	90	1.94376	1.65038	1.40294
42	2.11142	1.65692	1.30399	91	1.94190	1.65032	1.40415
43	2.10481	1.65663	1.30752	92	1.94007	1.65026	1.40535
44	2.09846	1.65635	1.31094	93	1.93828	1.65020	1.40654
45	2.09235	1.65609	1.31425	94	1.93651	1.65014	1.40770
46	2.08648	1.65584	1.31746	95	1.93478	1.65009	1.40885
47	2.08081	1.65559	1.32058	96	1.93308	1.65003	1.40998
48	2.07535	1.65536	1.32360	97	1.93140	1.64998	1.41109
49	2.07008	1.65514	1.32653	98	1.92975	1.64993	1.41219
50	2.06499	1.65493	1.32939	99	1.92813	1.64987	1.41327
51	2.06007	1.65473	1.33216	100	1.92654	1.64982	1.41433

Annex 7. Probabilistic modeling

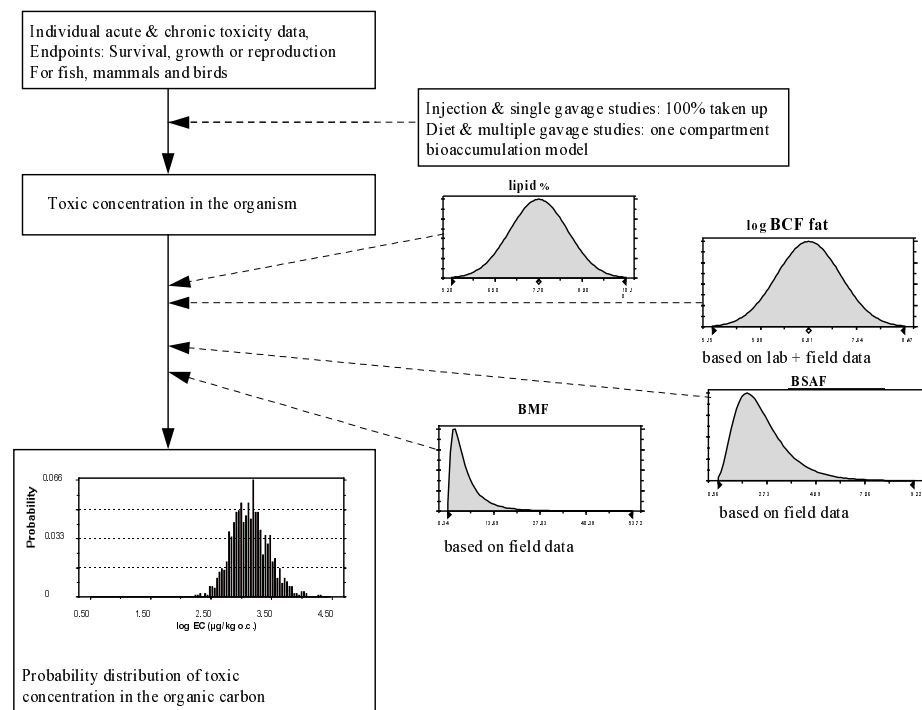
Probabilistic modeling is a new approach used for deriving ERLs for substances that accumulate through the foodchain, i.e. probabilistic foodweb modeling (Traas et al., 1996; Jongbloed et al., 1996; Van Wezel et al., 2000a). The approach as described by Van Wezel et al. (2000a) includes two major parts. First, all toxicity data for aquatic organisms, mammals and birds are recalculated into an equivalent toxic concentrations in (the organic carbon of) sediments or soils. For that reason biomagnification factors are included to recalculate the concentration from predator to food. BSAFs are included to recalculate the concentration from organism to the organic carbon of sediment or soil. In this way, all types of studies are readily compared on the same concentration axis and are integrated into one MPC. Second, probabilistic techniques are used to incorporate the spread in the data. Thus, probability distributions of sediment or soil concentrations associated with adverse effects are obtained. The contribution of the underlying parameters to the variance in the resulting probability distribution is also determined. MPCs are based on the 5th percentile of the combined distributions. The basis assumption is that the substances in the foodchain are in equilibrium with the organic carbon normalized concentration in the bed sediment.

Probability distributions can be fitted for all the toxicity data together, or for only the data on birds and mammals. This distinction is made to evaluate potential bimodal distributions, e.g. for example when aquatic species are far less sensitive than birds and mammals. The goodness-of-fit of the probability distributions is tested by the Kolgomorov-Smirnov test. If the s-value is lower than 0.1, the distribution is accepted as a valid to build the MPC upon. If not, the most sensitive probability distribution is chosen as a basis to derive the MPC.

The selected 5th percentiles are transformed into a concentration in mg/kg organic carbon content, and subsequently set as MPC. This procedure is analogous to the procedure as described by Aldenberg and Slob (1993), with the difference that probability distribution are used as the input instead of single values.

For a summary of the whole procedure as described in the preceding text, see Figure A7-1.

Step 1: recalculation of individual toxicity data into a probability distribution of the equivalent toxic concentration in the organic carbon of soil or sediment



Step 2: Combining the individual probability distributions

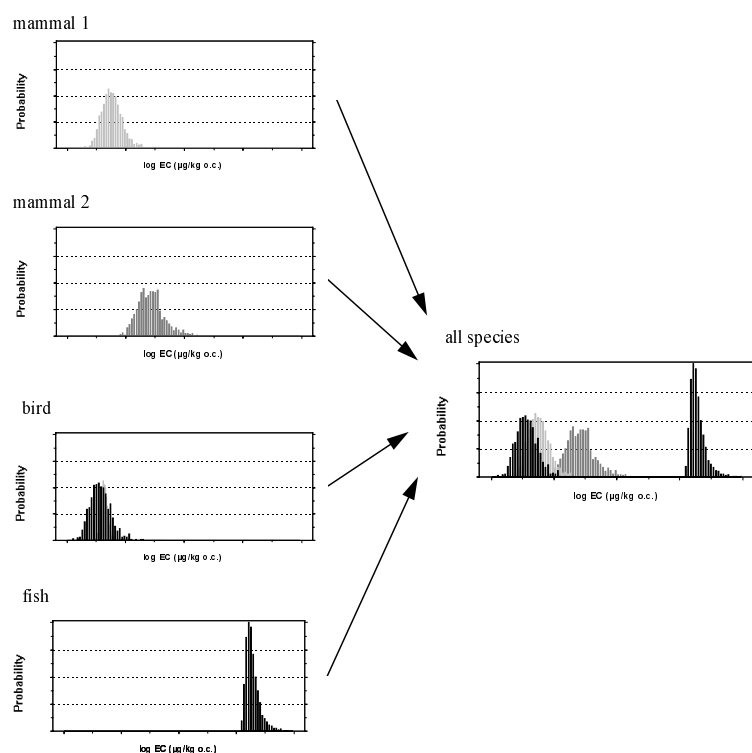


Figure A7-1. Overview on the different steps taken in the derivation of MPCs using probabilistic modeling with polychlorinated biphenyls as an example: Step 2 and 2 (below).

Annex 8. Qsars for aquatic toxicity of chemicals acting by narcosis

QSAR equations can be applied for chemicals acting by narcosis. The mechanism of narcosis is non-specific; the potency of a chemical to induce narcosis is entirely dependent on its hydrophobicity. This implies that, in the absence of all specific mechanisms of toxicity, a chemical will always be as toxic as its hydrophobicity (e.g. $\log K_{ow}$) indicates. Narcosis type toxicity is therefore also called 'baseline' toxicity or minimum toxicity. QSARs for chronic toxicity were selected for 19 aquatic species (Van Leeuwen et al., 1992, Verhaar et al., 1994). These are given in Table A8-1. From these QSARs, NOECs can be calculated for any $\log K_{ow}$ value. The MPC or $SRCECO$ can be calculated using Aldenberg and Jaworska (2000). By using the principles of Equilibrium partitioning, matching ERLs for sediment and soil can be calculated as well.

Table A8-1: QSARs for NOECs of selected species for chemicals acting by narcosis.

<u>Bacteria</u> Clostridium botulinum Bacillus subtilis Pseudomonas putida Photobacterium phosphorum	$\log NOEC = -0.82 \log K_{ow} - 0.29$ $\log NOEC = -0.64 \log K_{ow} - 2.03$ $\log NOEC = -0.64 \log K_{ow} - 1.60$ $\log NOEC = -0.68 \log K_{ow} - 1.52$
<u>Algae</u> Skeletonema costatum Scenedesmus subspicatus Selenastrum capricornutum	$\log NOEC = -0.72 \log K_{ow} - 1.42$ $\log NOEC = -0.86 \log K_{ow} - 1.41$ $\log NOEC = -1.00 \log K_{ow} - 1.71$
<u>Fungi</u> Saccharomyces cerevisiae	$\log NOEC = -0.78 \log K_{ow} - 0.35$
<u>Protozoans</u> Tetrahymena pyriformis	$\log NOEC = -0.80 \log K_{ow} - 1.28$
<u>Coelenterates</u> Hydra oligactis	$\log NOEC = -0.86 \log K_{ow} - 2.05$
<u>Molluscs</u> Lymnaea stagnalis	$\log NOEC = -0.86 \log K_{ow} - 2.08$
<u>Arthropods</u> Nitocra spinipes Daphnia magna Aedes aegypti Culex pipiens	$\log NOEC = -0.78 \log K_{ow} - 2.14$ $\log NOEC = -1.04 \log K_{ow} - 1.70$ $\log NOEC = -1.09 \log K_{ow} - 1.36$ $\log NOEC = -0.86 \log K_{ow} - 1.98$
<u>Fish</u> Pimephales promelas/ Brachydanio rerio	$\log NOEC = -0.87 \log K_{ow} - 2.35$
<u>Amphibia</u> Ambystoma mexicanum Rana temporaria Xenopus laevis	$\log NOEC = -0.88 \log K_{ow} - 1.89$ $\log NOEC = -1.09 \log K_{ow} - 1.47$ $\log NOEC = -0.90 \log K_{ow} - 1.79$

The HC5 is calculated under the assumption of a normal distribution of log toxicity data, according to the method of Aldenberg & Jaworska (2000) for narcotic chemicals as a function of K_{ow} . HC5-values are presented in Table A8-2 for $\log K_{ow}$ -values ranging from -1 to 7 at intervals of 0.1. Note, however, that due to a number of complicating factors the simple uptake and equilibrium partitioning models that were used for determining these values do not necessarily hold valid below $\log K_{ow} = 0$ and

above $\log K_{ow} = 5-6$. $\log K_{ow}$ values below 0 or above 6 are indicated bold italic in table (A8-2). Total water concentrations are based on a suspended matter content of 30 mg/l and an organic carbon content of 10%. Sediment concentrations are for a standard sediment with an organic carbon fraction of 0.0588 (cf. section 4.4.2 and 4.4.3) and an estimated K_{oc} (as described in Van der Kooij et al., 1991).

Table A8-2: log10 HC5 values for water, water with suspended matter (total) and sediment. Values for $\log K_{ow}$ below 0 or above 6 should be treated with caution.

logKOW	log HC5			logKOW	logHC5		
	dissolved mol/l	sediment mol/kg	total mol/l		dissolved mol/l	sediment mol/kg	total mol/l
-1.0	-1.68	-4.13	-1.68	3.1	-5.40	-3.75	-5.40
-0.9	-1.76	-4.11	-1.76	3.2	-5.50	-3.75	-5.50
-0.8	-1.84	-4.09	-1.84	3.3	-5.60	-3.75	-5.60
-0.7	-1.92	-4.07	-1.92	3.4	-5.70	-3.75	-5.70
-0.6	-2.00	-4.06	-2.00	3.5	-5.80	-3.75	-5.80
-0.5	-2.09	-4.04	-2.09	3.6	-5.90	-3.75	-5.90
-0.4	-2.17	-4.02	-2.17	3.7	-6.00	-3.75	-6.00
-0.3	-2.25	-4.01	-2.25	3.8	-6.10	-3.75	-6.10
-0.2	-2.34	-3.99	-2.34	3.9	-6.20	-3.75	-6.20
-0.1	-2.42	-3.97	-2.42	4.0	-6.30	-3.76	-6.29
0.0	-2.51	-3.96	-2.51	4.1	-6.40	-3.76	-6.39
0.1	-2.59	-3.95	-2.59	4.2	-6.51	-3.76	-6.49
0.2	-2.68	-3.93	-2.68	4.3	-6.61	-3.76	-6.59
0.3	-2.77	-3.92	-2.77	4.4	-6.71	-3.76	-6.69
0.4	-2.86	-3.91	-2.86	4.5	-6.81	-3.76	-6.79
0.5	-2.94	-3.90	-2.94	4.6	-6.91	-3.77	-6.88
0.6	-3.03	-3.89	-3.03	4.7	-7.02	-3.77	-6.98
0.7	-3.12	-3.87	-3.12	4.8	-7.12	-3.77	-7.07
0.8	-3.21	-3.86	-3.21	4.9	-7.22	-3.77	-7.16
0.9	-3.30	-3.85	-3.30	5.0	-7.32	-3.78	-7.25
1.0	-3.39	-3.85	-3.39	5.1	-7.43	-3.78	-7.34
1.1	-3.48	-3.84	-3.48	5.2	-7.53	-3.78	-7.42
1.2	-3.58	-3.83	-3.58	5.3	-7.63	-3.78	-7.50
1.3	-3.67	-3.82	-3.67	5.4	-7.74	-3.79	-7.57
1.4	-3.76	-3.81	-3.76	5.5	-7.84	-3.79	-7.64
1.5	-3.86	-3.81	-3.86	5.6	-7.94	-3.79	-7.70
1.6	-3.95	-3.80	-3.95	5.7	-8.05	-3.80	-7.76
1.7	-4.04	-3.80	-4.04	5.8	-8.15	-3.80	-7.81
1.8	-4.14	-3.79	-4.14	5.9	-8.25	-3.81	-7.86
1.9	-4.23	-3.79	-4.23	6.0	-8.36	-3.81	-7.90
2.0	-4.33	-3.78	-4.33	6.1	-8.46	-3.81	-7.94
2.1	-4.42	-3.78	-4.42	6.2	-8.57	-3.82	-7.97
2.2	-4.52	-3.77	-4.52	6.3	-8.67	-3.82	-8.00
2.3	-4.62	-3.77	-4.62	6.4	-8.77	-3.83	-8.02
2.4	-4.71	-3.77	-4.71	6.5	-8.88	-3.83	-8.04
2.5	-4.81	-3.76	-4.81	6.6	-8.98	-3.83	-8.06
2.6	-4.91	-3.76	-4.91	6.7	-9.09	-3.84	-8.07
2.7	-5.01	-3.76	-5.01	6.8	-9.19	-3.84	-8.09
2.8	-5.10	-3.76	-5.10	6.9	-9.30	-3.85	-8.10
2.9	-5.20	-3.76	-5.20	7.0	-9.40	-3.85	-8.11
3.0	-5.30	-3.75	-5.30				

Annex 9. Documentation requirements

Below, minimum requirements are formulated for documenting derived ERLs. These requirements do not specify the exact report format, since this may vary according to available templates or styles, and the specific study that is documented. The order and subdivisions of paragraphs may vary as well, depending on the case-study.

A9.1 Summary/*Uitgebreide samenvatting*

The summary (and the 'uitgebreide samenvatting' in Dutch) should report the methodology that was used to calculate the ERLs (Section 6). Tables are provided reporting the NC, MPC and SRC_{ECO} for the compartments water, soil, sediment and groundwater (with units provided). ERLs for water compartments should be reported for both dissolved and total concentrations (cf. table 13) and report if specific values are derived for saltwater.

If previously derived ERLs exist, these should be reported as well.

In addition, the final BCFs and K_p values used for derivation of ERLs (for secondary poisoning and the Equilibrium Partitioning method) are reported.

A9.2 Introduction

The introduction should report the government agency that commissioned the work and the expert panel procedures employed to guide the derivation of ERLs.

References are made to existing overviews of ERLs and guidance documents.

Deviations of the case-study with respect to current methodology should be introduced.

A9.3 Properties and use

This section reports the basic properties, use, production and discharge of the compound. This is necessary for an adequate risk assessment and allows (other) risk assessors to use the basic data for their purpose, e.g. EUSES calculations.

A9.3.1 Physico-chemical properties

The following properties should be reported (if available, cf. Van Wezel and Van Vlaardingen, 2001):

Property	Value(s)	Reference
IUPAC Name		
CAS number		
EINECS number		
Structural formula (diagram)		
Empirical formula		
Molar Mass		
n-Octanol/water partition coefficient (K _{ow})		
Soil/sediment water sorption coefficient (K _{oc})		
Solubility		
Melting Point		
Vapour Pressure		
Henry's law constant		
pK values (dissociation constant)		

A9.3.2 Use, production and discharge

The use, toxic mode of action (TMoA), production volumes and discharge of a compound should be reported if available. This information can be sourced from recent reviews or (monitoring) reports.

A9.4 Methods

A9.4.1 Data Search

The method section should report the search strategy to acquire toxicity data, mention previous relevant sources of data such as previous RIVM report, WHO environmental health criteria, EPA reports, etc. If additional data were acquired such as Kp's, BCFs or BSAFs the strategy should be reported as well.

A9.4.2 Derivation of ERLs

The methods used for derivation of ERLs are reported. When standard methodology is used, this may be brief with reference to guidance documents or published methods. Essential equations should be provided. Deviations or extensions must always be reported in full, using equations with full specification of units employed.

A9.5 Results and Discussion

A9.5.1 Data and analysis

The collected data and subsequent analysis are reported. If variability in data is observed, histograms or distributions and regressions of data against environmental/chemical factors might help interpretation (e.g. Smit et al., 2000).

A9.5.2 Specific problems/properties

Specific factors that influence toxicity are reported and discussed such as toxic mode of action (TMoA), bioavailability, degradation, hydrolysis, bioaccumulation, biotransformation, congener –specific toxicity etc (see e.g. Van Wezel et al., 1999).

A9.5.3 Derivation of ERLs

For each compound in a case study, the method of derivation is reported including the data used for calculating the ERLs. In the case of refined risk assessment, the data and fitted distribution are depicted (see e.g. Verbruggen et al., 2000). If data are subdivided, such as for salt and freshwater toxicity data or target vs. non-target organisms, subdivisions should be shown preferably in the same graph.

An overview table of all ERLs derived in the report is presented. A reference is made to an Annex with ***mean, standard deviation and number of observations*** for each case where refined risk assessment is applied.

A9.6 Preliminary Risk Analysis

A.9.6.1 Multiple species /(semi)field experiments

If data from (semi)field testing are available, such as micro- or mesocosm tests or field tests with agrochemicals, a comparison of derived ERLs with NOECs derived from such experiments is performed. Examples of such comparisons can be found e.g. Crommentuijn et al., 1997b and Versteeg et al., 1998. The main goal is to establish if

the derived ERLs are protective to ecosystems. As seems generally true; ERLs seem to represent a lower confidence limit of NOECs for (microcosm) ecosystems (Versteeg et al. (1998).

A9.6.2 Concentrations

This section reports environmental concentrations found in surface water, sediment and soil. In general, most monitoring data concern aquatic concentrations. If monitoring data for the Netherlands is available (RIKZ, RIZA or RIVM), the distribution of concentrations over a (or several) year(s) is preferably shown, together with a distribution describing the data. Data from other countries can be shown if data for the Netherlands is lacking.

In many cases, it can be expected on theoretical grounds that environmental concentrations follow a log-normal distribution. From the data, the mean, median, SD, and the 90th percentile value are reported. The 90th percentile value of the distribution may be derived directly from the data (if the data set is large) or from the fitted distribution. Statistical analysis of the data sets (e.g. if certain rivers or reaches are more polluted than others) may be employed to provide additional information (e.g. Kalf and van den Hoop, in prep.).

The number of locations where the 90th percentile is exceeded (for time-averaged values, e.g. Crommentuijn et al., 1997b), or the frequency of exceedance of the 90th percentile (for monitoring data, e.g. Kalf and Van den Hoop, in prep.) are reported.

A9.6.3 Preliminary risk analysis

This section reports a preliminary risk analysis, preferably based on a comparison of the 90th percentiles of (monitoring) data and the derived ERLs (e.g. Kalf and van den Hoop in prep.). The choice for the 90th percentile is based on the notion that peak concentrations are relevant for determining ecological risk, even though the frequency of occurrence is much lower than the average concentrations. If 90th percentiles of data are higher than derived ERLs, ecotoxicological effects may be expected, depending on the type of ERL that is exceeded. In general, ecotoxicological risk is expected to occur above the MPC. Serious risks are expected if the SRC_{ECO} is exceeded.

A9.7 Conclusions and recommendations

This section combines the main conclusions and recommendations.

A9.8 Data tables

The data used for deriving ERLs are tabulated and reported in Annexes (cf. Section 5). The main data tables are toxicity data, bioaccumulation data (BCF, BAF, BSAF), partition coefficients and the final (recalculated) data used for derivation of ERLs.

Annex 10. Calculation of ERLs for total water concentrations

A10.1 Organic compounds

The MPCs for dissolved organic compounds in water can be recalculated to the total water phase, based on differences in the content of organic matter. The following equation is used to calculate the $MPC_{water,total}$:

$$MPC_{water,total} = MPC_{water,dissolved} (1 + K_{ppm} \times 0.001 \times 0.03)$$

With 0.001 = conversion constant [g/kg]
 0.03 = content of suspended matter (g/l) (considered the standard)
 K_{ppm} = partition coefficient suspended matter/water,

K_{ppm} is calculated from the K_p sediment/water or from the K_{oc} . Suspended matter is standardised at an organic matter content of 20% (or organic carbon content of 11.72 %), twice as high as standardised soil or sediment (cf. section 4.4.3). This means that the K_{ppm} is twice as high as the K_p for sediment/water. If the K_p sediment/water is estimated from the K_{oc} , the following equation applies (cf. 4.4.2) for suspended matter as well:

$$K_{ppm} = K_{oc} * f_{oc} \quad (A11-1)$$

in which:

K_{ppm} = partition coefficient for standard suspended matter [l/kg]
 K_{oc} = organic carbon-normalised partition coefficient [l/kg]
 f_{oc} = fraction organic carbon (0.1172 [g oc/ g dw suspended matter])

The $NC_{water,total}$ is defined as the $MPC_{water,total} / 100$.

A10.2 Metals

MPCs for metals consist of the Maximum Permissible Addition (MPA) and the background concentration. To recalculate the MPCs from dissolved water concentrations to total water concentrations (or vice-versa), partition coefficients are used. These are applied only to the non-background part, i.e. the background concentration is subtracted. After recalculation, the background concentration (C_b) is added again. The recalculation is performed as:

$$MPC_{water,total} = MPC_{water,dissolved} - C_{b,dissolved} + (MPC_{water,dissolved} - C_{b,dissolved}) \times K_{ppm} \times 0.001 \times 0.03 + C_{b,dissolved}$$

with $C_{b,dissolved}$ = dissolved background concentration
 K_{ppm} = partition coefficient suspended matter/water [l/kg]
 0.001 = conversion constant [g/kg]
 0.03 = standardised content of suspended matter (g/l)

The K_{ppm} is calculated from the K_p sediment/water, by multiplying the K_p sediment/water by a factor of 1.5. This is mainly due to the higher clay content of

standard suspended matter, set at 40%. The clay content of standard soil or sediment is set at 25% (cf. section 4.4.3).

NCs for metals consist of the Negligible Addition (NA) and the background concentration. To recalculate the NCs from dissolved water concentrations to total water concentrations (or vice-versa), partition coefficients are used. These are applied only to the non-background part, i.e. the background concentration is subtracted. After recalculation, the background concentration (C_b) is added again. The recalculation is performed as:

$$NC_{\text{water,total}} = NC_{\text{water,dissolved}} - C_{b,\text{dissolved}} + (NC_{\text{water,dissolved}} - C_{b,\text{dissolved}}) \times K_{\text{ppm}} \times 0.001 \times 0.03 + C_{b,\text{dissolved}}$$

with

$C_{b,\text{dissolved}}$ = dissolved background concentration
 K_{ppm} = partition coefficient suspended matter/water [l/kg]
 0.001 = conversion constant [g/kg]
 0.03 = content of suspended matter (30 mg/l) (considered the standard)

Annex 11: Derivation of MPCs in air for humans and harmonisation¹

A11.1 Derivation of MPCs in air for humans

Until now, MPCs for humans have only been derived for volatile compounds like non-halogenated monocyclic aromatic hydrocarbons (e.g. benzene, styrene, toluene), halogenated monocyclic aromatic hydrocarbons (e.g. chlorobenzenes) and aliphatic chlorinated hydrocarbons. Due to their volatility, it is assumed that exposure of humans via air is a more important route than for ecosystems. The contribution of possible exposure through other routes is not taken into account. Therefore, a MPC_{HUMAN}² for volatile compounds has only been derived for the compartment air.

A minimum toxicity data set is defined that has to be met in order to derive an MPC for man (Rademaker et al., 1993a). According to this minimum set, information on the following aspects is required:

- (sub)chronic toxicity
- carcinogenicity
- mutagenicity
- teratogenicity
- reproductive toxicity.

If data are used from reproduction studies, the studies should in principle cover the whole reproduction cycle from sexual maturity to growth and development of the following generations. The dataset is complete if one or more toxicity tests are available on the five items mentioned. Out of these toxicity tests the most critical study is selected. Concerning the volatile compounds, the exposure route of the most critical study has to be inhalation. Oral studies are only accepted for completing the minimum data set of the compound, i.e. an MPC cannot be based on an oral study. However, if for instance it is concluded from an oral teratogenicity study that the compound is not teratogenic, no inhalatory study has to be available. In addition to laboratory toxicity tests with mammals, epidemiological studies can be used for the derivation of an MPC. For the derivation of an MPC for humans, a distinction is made between non-carcinogenic and carcinogenic compounds.

1. All selected NOECs and LOECs are corrected for continuous exposure (see formula 13, section 4.4.4). This results in duration-corrected values (DCVs).
2. The lowest DCVs are selected for further consideration with respect to aspects such as relevance of parameters studied and animal species and the progression of the various effects in time.
3. An MPC is calculated from the most relevant DCV by applying uncertainty factors (UFs). UFs of 10 x 10 for interspecies and intraspecies variation are

¹ This section is an excerpt from De Bruijn et al., 1999

² In the more recent terminology of section 6.7, The human toxicological risk limit is the Maximum Permissible Risk (MPR) that corresponds to Maximum Permissible Concentrations in environmental compartments.

always applied. The magnitude of other UFs, for extrapolation from subchronic to chronic exposure or from LOEC to NOEC, depends on the toxicological profile of the compound. Aspects like type of effect (nature, severity and biological significance), specificity of the study, progression of the effect in time, duration of the study and extent of available information on the compound determine the height of the UF.

A11.2 Carcinogenic compounds

For genotoxic carcinogens a linear non-threshold cancer risk model is used for deriving an MPC. This model uses the tumour incidence scheme from chronic animal studies as a starting point (VROM, 1984). The MPC is defined as 10⁻⁶/year meaning that the annual probability of mortality due to the occurrence of cancer is 1 in a million (VROM, 1989b).

If one or more elements of the minimum toxicity data set are lacking, a preliminary MPC for humans is derived (Rademaker et al., 1993b). For deriving a preliminary MPC the UFs used for extrapolation of the most critical study are applied more conservatively: the UFs for interspecies and intraspecies variation, for extrapolation from sub-chronic to chronic exposure and for converting a LOEC to NOEC are all equal to 10. NOECs or LOECs from teratogenicity tests are extrapolated with an extra factor 10 for teratogenic effects, but the UF for exposure time is not applied. Also, an oral study can be used as the principal study for extrapolation. Therefore oral NOECs or LOECs are converted to inhalatory ones using formula 13 (see section 4.4.4).

A11.3 Procedure to derive MPCs for the air compartment

Because the aim of an MPC is to protect all organisms against adverse effects (direct and indirect) due to exposure of substances, depending on the compartment, both ecotoxicological and human toxicological data have to be taken into account to set an MPC. The MPCs for air derived until now are based on the human effect assessment as described in the previous section (Rademaker et al., 1993a,b). If relevant data are available, an assessment of the effects on the ecosystems is made and the result is compared to the human effects assessment. In addition, for metals and for some organic substances so-called critical air concentrations are calculated. These critical air concentrations give the steady-state concentrations in air at which the MPC in natural soil will not be exceeded. Hence, these values can e.g. be used to evaluate if emissions to air, leading to certain air concentrations, provide the necessary protection for soil ecosystems in the long term.

In order to harmonise the quality criteria for water and soil the equilibrium partitioning concept is applied (cf. section 6.5). This concept is not to be applied for the harmonisation of water and soil quality criteria with criteria for air. Due to the rapid refreshment of the atmosphere, concentrations in air on the one hand and water and soil on the other hand will not approach equilibrium. Therefore, it is proposed to apply computed steady-state concentration ratios, rather than equilibrium concentrations as a basis for harmonisation between air on the one hand and soil and water on the other hand (Van de Meent and de Bruijn, 1995).

A11.4 Harmonisation of MPCs for air, water and soil

A multimedia box model calculation is used to estimate the steady-state intermedia concentrations that are expected to be the long-term result of the present environmental management policy. Comparison of these computed intermedia concentration ratios with the ratios of the MPCs will indicate if co-existence of the proposed concentration levels is achievable in practice. In the next sections this procedure will be described in more detail.

A11.4.1 The SimpleBox model

The steady-state concentrations in air, water sediment and soil are calculated with the model SimpleBox. SimpleBox is a multi-media fate model commonly referred to as a 'Mackay type' box model (Van de Meent, 1993). The environmental compartments are represented by homogeneous boxes. The concentration of a chemical in these boxes is affected by processes that cause mass flows of the chemical to and from the boxes. For the purpose of harmonisation of MPCs, SimpleBox represents the behaviour of micropollutants in a model environment, resembling the Netherlands.

A schematic representation of the model is shown in Figure A11.1 in which all the transport routes of the chemical from one compartment to another are presented as arrows. A detailed description of these transport routes is given in section A11.7. The main characteristics of the reference environment (in this case the Netherlands) are also given in this appendix. The model environment consists of eight homogeneous compartments: air, surface water, suspended particles, sediment, aquatic organisms and three soil compartments. These three separate soil compartments are defined to mimic the many different soil types and differences in soil use in the Netherlands. The first soil compartment represents 'natural soil'. The relevant characteristic of this compartment is that only one route of entry of chemicals exists into this compartment, namely exchange with the atmosphere. The second soil type represents 'agricultural soil'. In addition to atmospheric input, this compartment may also be loaded directly, e.g. by fertilizer. The third soil compartment, 'industrial soil', is used to reflect the existence of 'urban' or 'industrial' soil.

In order to run SimpleBox several physico-chemical properties of the substance are needed. The most important ones are the vapour pressure and water solubility (or Henry's law constant derived from them), the soil/water partition coefficient including octanol/water partition coefficient, and degradation rates in air, water, and soil. The selection of these data is described in De Bruijn et al. (1999, Annex 1).

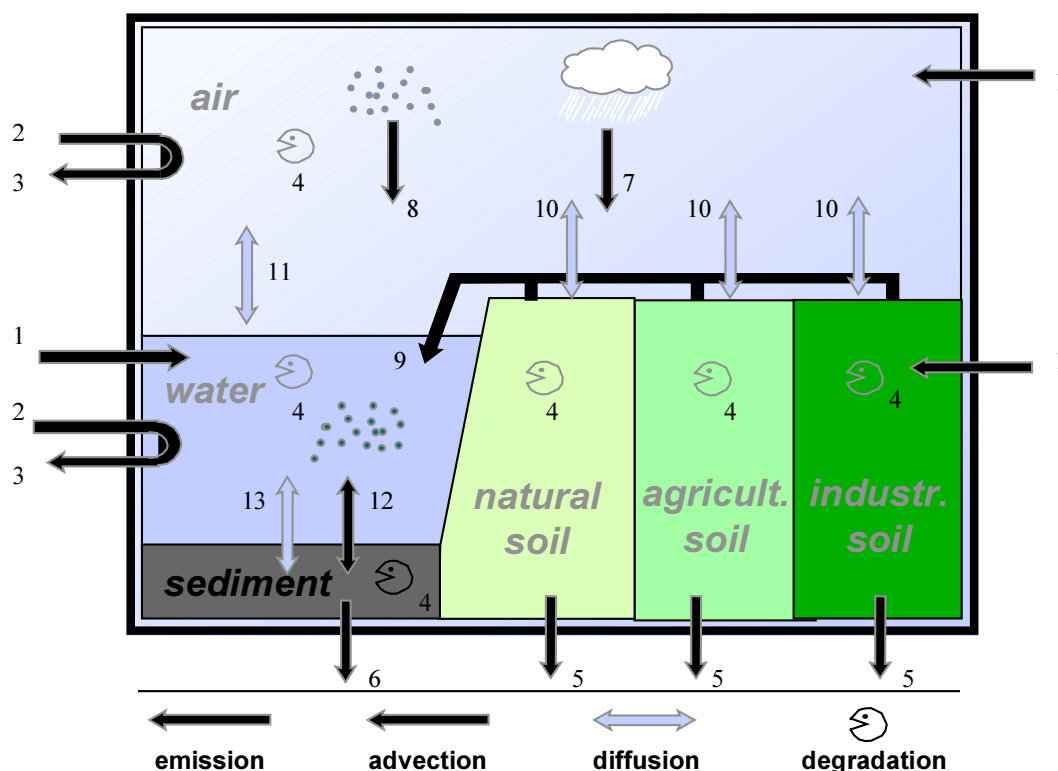


Figure A11.1: Schematic representation of the Simplebox model used to calculate steady-state concentrations. Explanation: 1= emission, 2= import, 3= export, 4= degradation, 5= leaching, 6= burial, 7= wet deposition with rain, 8= dry deposition with aerosols, 9= run-off, 10= air-soil exchange through gas absorption and volatilization, 11= air-water exchange through gas absorption and volatilization, 12= sedimentation and resuspension, 13= sediment-water exchange through direct sorption and desorption.

A11.5 Harmonisation Procedure

When the individual MPCs for the different compartments have been derived and the physico-chemical data are collected, the harmonisation of the MPCs can be carried out. The objective of the harmonisation procedure is to compare the concentrations at steady-state in the receiving compartments (also called the secondary compartments) with the MPCs that have been derived for these compartments from (eco)toxicological data. If this comparison indicates that maintaining the concentration in the primary compartment (the compartment of emission) at MPC level results in exceeding the MPC in any of the secondary compartments, the set of MPCs must be considered incoherent and has to be adjusted. The harmonisation procedure on the base of the SimpleBox model is developed by Van de Meent and De Bruijn (1995). This stepwise procedure consists of the following steps:

Step 1: Determination of the primary compartment

First it is assumed that emissions of the chemical take place exclusively into one of the compartments air, soil or water. It is also assumed that these emissions lead to concentrations similar to the MPC for this primary compartment. Data from the Dutch Emission Registration and several reports containing information on the emission of chemicals are used to determine the compartments into which chemicals are released

(primary compartments). If a chemical is released into more than one compartment, the calculations have to be repeated.

Step 2: Calculation of the equilibrium concentrations in the secondary compartments

Equilibrium concentrations are considered as maximum achievable concentrations in the secondary receiving compartment. Concentrations higher than the equilibrium concentration are possible if intermedia transport is dominated by mechanisms such as atmospheric deposition or sedimentation.

When the concentration in the primary compartment is assumed to be equal to the MPC derived for that compartment, the equilibrium concentrations in the secondary compartments can be calculated according to the following equilibrium partitioning relationships:

$$\frac{C_{air}}{C_{water}} = \frac{H_c}{R \cdot T} \cdot 1000 \quad (A11-1)$$

$$\frac{C_{soil}}{C_{water}} = Kp_{soil} \quad (A11-2)$$

$$\frac{C_{air}}{C_{soil}} = \frac{H_c}{R \cdot T \cdot Kp_{soil}} \cdot 1000 \quad (A11-3)$$

with:

C_{air}	= concentration in air (mg/m ³)
C_{water}	= concentration in water (mg/l)
C_{soil}	= concentration in soil (mg/kg)
H_c	= Henry's law constant (Pa.m ³ /mol)
R	= gas constant (8.314 Pa.m ³ /mol.K)
T	= temperature (K)
Kp_{soil}	= soil-water partition coefficient (l/kg)

Step 3: Comparison of the equilibrium concentrations in the secondary compartments with the MPCs for these compartments

When the equilibrium concentrations in the secondary compartments have been calculated these concentrations are compared to the MPCs derived for the corresponding compartments. Two different situations may arise:

1. The equilibrium concentrations in the secondary compartment(s) are lower than the MPCs in these compartments. Because the equilibrium concentrations can be regarded as the maximum achievable concentrations, it can be concluded that the MPC of the primary compartment will never cause exceedance of the MPCs for the secondary compartments. Thus, the MPCs in water, soil and air can be considered as a coherent set of values.

2. The equilibrium concentrations in the secondary compartments are higher than the MPCs derived for these compartments. This indicates that the MPC in the primary compartment can cause adverse effects in the secondary compartments. However, due to intermedia transport it may well be possible that the equilibrium concentration will not be reached in the secondary compartment(s). In this case it is necessary to calculate the steady-state concentration with the SimpleBox model.

Step 4: Calculation of the steady-state concentrations in the secondary compartments by SimpleBox and comparison with MPCs for these compartments

To test if the MPCs for the different compartments meet the coherence-criterion, SimpleBox is run, assuming that the emission in the primary compartment is such that the concentration becomes equal to the MPC. Input by import is treated as follows: concentrations of the chemical in the primary compartment outside the system (import) are assumed to be equal to the MPC (Figure A11.1, arrow 2), while concentrations in the secondary compartments are set equal to zero. For example, when water is the primary compartment, the concentration in water imported in the system is equal to the MPC in water, whereas the concentration in imported air is zero. When the steady-state concentrations in the secondary compartments have been calculated two different situations are possible:

1. The steady-state concentration is lower than the MPC: adjustment of the MPC of the primary compartment is not necessary. The MPCs for the different compartments can be regarded as a coherent set of values;
2. The steady-state concentration exceeds the MPC: the MPC of the primary compartment should be adjusted downwards to a value that will not lead to problems in the secondary compartments.

Based on a sensitivity analysis it was concluded that it seems reasonable to assume an uncertainty factor of 10 for the outcome of the calculations with SimpleBox (Van de Plassche and Bockting, 1993). Therefore, it was decided to adjust the MPC of the primary compartment only if the steady-state concentration in the secondary compartment exceeds the MPC in this compartment by more than a factor 10. For example; when a substance is emitted to water and the calculated steady-state concentration in air is 8 times higher than the MPC derived for air (secondary compartment), no adjustment of the MPC in water is necessary. However, when the steady-state concentration in air is more than 10 times higher than the MPC in the secondary compartment, adjustment of the former value will take place in steps of 10: e.g. if the steady-state concentration in the secondary compartment is 10-20 times higher than the MPC for the corresponding compartment, the MPC for the primary compartment has to be adjusted downwards with a factor 10. Consequently, if the MPC in sediment is based on equilibrium partitioning, this value must also be adjusted.

The conclusion that one of the MPCs of the compartments air, water or soil has to be adjusted in order to prevent exceedance of the MPCs in the secondary compartments

depends not only on the outcome of the model calculation. The basis for the MPCs themselves also has to be taken into account. If high safety factors are applied to set the MPC because of insufficient knowledge on the effects of the chemical it is questionable whether the MPC of a secondary compartment must be adjusted because of the fact that the steady-state concentration exceeds the MPC. This assessment, however, has to be made on a case by case basis.

This procedure for harmonisation of MPC values for air, water and soil (Van de Meent and de Bruijn, 1995) has been applied to some 30 volatile organic chemicals (Van de Plassche and Bockting, 1993).

A11.6 Calculation of critical air concentrations

For most compounds no ecotoxicological data are available to calculate an MPC for air. Although emissions to air for other than the volatile compounds can be substantial, risk levels for air are therefore often lacking, making it impossible to assess the risks of these emissions. However, the procedure described in this chapter gives the opportunity to calculate so-called 'critical air concentrations' without using ecotoxicological data (Van de Meent, 1995; Traas et al., 1996). 'Critical' here means that these steady-state concentrations in air and rain water will in the long term not lead to exceedance of the environmental quality criteria for soil. Steady-state soil/air concentration ratios (SSCR) are calculated using the SimpleBox model. From this SSCR it is possible to calculate the Critical Air Concentration (CritCONC_{air}) and the Critical Concentration in rain water (CritCONC_{rain}) using the following formulas:

$$CritCONC_{air} = \frac{MPC_{soil}}{SSRC_{soil/air}} \quad (A11-4)$$

and

$$CritCONC_{rain} = CritCONC_{air} \cdot ScavRatio \quad (A11-5)$$

with:

- CritCONC_{air} = critical concentration in air in g/m³
- MPC_{soil} = maximum permissible concentration in soil in g/kg (dry weight)
- SSCR_{soil/air} = steady-state concentration ratio soil/air in m³/kg (dry weight)
- CritCONC_{rain} = critical concentration in rain water (mg/l)
- ScavRatio = scavenging ratio, i.e. the ratio of the concentration in rain water and air in m³/m³

The SimpleBox model is originally developed for organic substances. Application of the model for metals in order to calculate SSCRs is possible but needs specific parameter settings for log K_{ow}, vapour pressure, scavenging ratio, fraction aerosol bound metal and degradation rates (cf. Traas et al., 1996).

A11.7 Transport Routes And Main Characteristics Of The Simplebox Model

Several transport routes of the chemical from one compartment to another are possible. For technical specifications is referred to Van de Meent (1993). A short description of the transport routes, presented in Figure A11.1 is given below:

- Input of the chemical into the system takes place by emission (arrow 1) into the compartments air, water, suspended matter, soil 2 and soil 3.
- The air, water and suspended matter are continuously being renewed by air and water from “outside”. This leads to an import (arrow 2) and export (arrow 3) of chemicals to and from the system. The export of the chemical (with air, water and suspended matter) is controlled by a residence time of the medium.
- Air-water exchange by gas adsorption and volatilization (arrow 11) is modeled by means of the classical two-film approach. Diffusive air-soil (arrow 10) and sediment-water exchange (arrow 13) are modeled similarly.
- Atmospheric deposition is the summation of three mechanisms: dry deposition of aerosols (arrow 8), gas phase wash-out by rain (arrow 7) and wet particle scavenging; dry deposition by gas absorption, which is often included as an atmospheric deposition term, is treated separately here. The gas, rain water and aerosol phases in air are at equilibrium.
- Sedimentation and resuspension (arrow 12): the assumption is made that there is no equilibrium between water and suspended matter. Instead, the exchange between suspended matter and water is regarded as a kind of first order process with an equilibration half time of 10 hr. The net sedimentation is deduced from the difference in concentrations of suspended matter between the incoming and outgoing water.
- Run off (arrow 9) from soil to surface water and vice versa.
- Burial of the chemical (arrow 6) in old sediment is controlled by the net sedimentation rate.
- The mass flow due to leaching (arrow 5) is derived by assuming that 40% of the total wet precipitation infiltrates into the soil and that the percolate is at equilibrium with the solid phase of the soil.
- Degradation (arrow 4) is characterized by pseudo first order rate constants (one for each compartment).
- Bioaccumulation in aquatic organisms.
- Adsorption from the aquatic phase to sediment (arrow 13) or suspended matter.

The main characteristics of the reference environment (in this case the Netherlands) that are used in the SimpleBox model, are given in the following table:

system area	37,925	atmospheric residence time	0.51 d
area % water	12.5%	wet precipitation	760 mm/yr
area % soil 1	41.5%	particle scavenging factor	$2 \cdot 10^5$
area % soil 2	45%	deposition velocity aerosols	0.1 cm/s
area % soil 3	1%	hydraulic residence time	53.1 d
mixing height air	1,000 m	settling velocity suspended particles	2.5 m/d
depth water	3 m	net sedimentation rate	0.3 mm/yr
concentration suspended matter	15 mg.l^{-1}	fraction soil infiltration	40%
mixing depth sediment	3 cm	fraction soil run-off	0%
mixing depth soil 1	5 cm		
mixing depth soil 2	20 cm	susp-water equilibration half time	10 hr
mixing depth soil 3	5 cm	mass transfer air side air-water interface	$1.4 \cdot 10^{-3} \text{ m/s}$
organic carbon content suspended matter	10%	mass transfer water side air-water interface	$1.4 \cdot 10^{-5} \text{ m/s}$
organic carbon content sediment	5%	mass transfer water side water-sed interface	$2.8 \cdot 10^{-7} \text{ m/s}$
organic carbon content soil 1	5%	mass transfer water side water-sed interface	$1.8 \cdot 10^{-7} \text{ m/s}$
organic carbon content soil 2	5%	mass transfer air side air-soil interface	$1.4 \cdot 10^{-3} \text{ m/s}$
organic carbon content soil 3	5%	mass transfer soil air side air-soil interface	$5.6 \cdot 10^{-6} \text{ m/s}$
Temperature	12°C	mass transfer soil water side air-soil interface	$5.6 \cdot 10^{-10} \text{ m/s}$

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