Preface

This report "Environmental Risk Limits in The Netherlands" provides an overview of the risk limits, i.e. Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) in surface water, soil, air, groundwater and sediment for approximately 200 substances. The present report from the Dutch National Institute of Public Health and the Environment (RIVM), contains risk limits from the last decade obtained in the framework of the project "Setting Integrated Environmental Quality Standards". Deriving environmental risk limits should be a procedure which is transparent to all parties involved and from which different parties can benefit. Earlier RIVM-reports on environmental risk limits did not include all the underlying (ecotoxicological) data or all the methods that were used to derive environmental risk limits. That information was published in separate reports. The objective is to present the procedures to derive the environmental risk limits, the risk limit values themselves and all underlying data used for the derivation of these limits. Risk limits are further used in the Dutch environmental policy as the foundation of the environmental quality standards. The latter are described in the policy document: "Setting Integrated Environmental Quality Standards: environmental quality standards for soil, water & air" (1999).

I would like to acknowledge the enormous help that the agency **HASKONING Consulting Engineers and Architects** provided us with in compiling and finalizing this report. I especially thank Mrs. E.P. van der Zande-Guinée, Ms. I.M.C. van Renesse and Mr. M.T. de Kok for their valuable and professional contribution.

Additional copies of this report (report no. 601640 001) cost Dfl 70 for Parts I to III and Dfl 185 for Part IV. These copies can be obtained from the Library of the National Institute of Public Health and the Environment.

I hope that this report will be useful to you,

Dr. H. Könemann

Head, Centre for Substances and Risk assessment (CSR)
National Institute of Public Health and the Environment (RIVM)

Readers guide

The objective of this report "Environmental Risk Limits in The Netherlands" is to present to interested parties involved in environmental policy or environmental risk assessment of chemical substances the procedures to derive the environmental risk limits. The report provides an overview of the risk limits, i.e. Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for approximately 200 substances.

The present report consists of four parts. Part I 'Procedure' describes the currently applied procedures to derive environmental risk limits. In Part II 'Risk limits' these procedures are applied to approximately 100 substances. For every substance a summary of the available data and the resulting harmonized MPC and NC values is given. The references that are used are listed separately following the substance descriptions. These substances are categorized as follows:

- A. Monocyclic aromatic hydrocarbons;
- B. Polycyclic aromatic hydrocarbons;
- C. Aliphatic hydrocarbons;
- D. Pesticides.

In Part III 'Data' all toxicological and ecotoxicological data are listed that have been used to derive the MPCs. These data are first categorized into the above mentioned groups, listed per substance and further categorized per environmental compartment. In addition, the toxicological and ecotoxicological data for metals that are not included in the enclosed report on metals (Crommentuijn et al., 1997^a) are listed in Part III.

In the fourth part, named **RIVM Report**, you will find the most recent reports on MPCs and NCs for metals (Crommentuijn et al., 1997^a), pesticides (Crommentuijn et al., 1997^b) and anilines (Reuther et al., 1998).

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ENVIRONMENTAL RISK LIMITS IN THE NETHERLANDS

**Jack de Bruijn, Trudie Crommentuijn, Kees van Leeuwen, Erik van der
Plassche, Dick Sijm, Martine van der Weiden**

Part I. PROCEDURE

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1. INTRODUCTION

1.1 Background

As described in the third National Environmental Policy Plan (NEPP, 1998) environmental policy in The Netherlands combines two approaches: a source-oriented track and an effects-oriented track. The **source-oriented** policy aims at reducing emissions of (potentially) hazardous substances from point and diffuse sources by applying best available technology (point sources) or best environmental practice (diffuse sources). Requirements on these sources can generally be imposed by the licensing authorities. The government has formulated in the first NEPP (NEP, 1990) some general premises underlying the source-oriented policy:

- unnecessary environmental pollution should be avoided;
- stand-still principle, i.e. no further damage to the environment;
- abatement at source is preferred above treatment at a later stage.

In essence, source-oriented environmental standards for substances are emission standards. However, since the source-oriented approach is not primarily connected with the possible effects that substances may have on the environment, it cannot be guaranteed that there will be no environmental damage when all the requirements are met. The techniques available and applied may not result in sufficient emission reductions or there may be other sources, possibly abroad, that are overlooked. There might be a burden from the past. Hence, there is also a need for an **effects-oriented** approach. The effects-oriented approach uses environmental quality standards and compares these with the concentrations of a substance in the different environmental compartments. If these effects-oriented standards are exceeded, (extra) requirements may be imposed on the sources which go beyond the requirements based on the premises of the source-oriented approach. Hence, effects-oriented quality standards can act as tools for the evaluation of the source-oriented measures.

Sustainable development is the general basis of the overall environmental policy as defined in the NEPP (NEPP, 1990). Sustainable development means that the quality of the environment is guaranteed for the next generation and beyond. In other words, that exposure to substances should not result in 'adverse' effects on man and ecosystems. Clearly, this assumption will only hold true if the effects-oriented standards act as a safety net for substances which cannot be controlled adequately through the source-oriented policy.

1.1 Risk Limits

The derivation of environmental quality standards to be used in Dutch environment policy is carried out in the project 'Setting Integrated Environmental Quality Standards' and is based on a risk policy. This risk policy does not only focus on the health and well-being of human beings but also on the ecosystem (environmental functions and nature values). The policy document 'Premises for Risk Management (1988)' provides the basis for setting standards for the concentration of a substance or a group of substances in the environmental compartments. For all environmental compartments substance concentrations can be calculated below which the occurrence of adverse effects is considered to be negligible: the **Negligible Concentration (NC)**. There is also a concentration above which the risk of such effects is unacceptable: the **Maximum Permissible Concentration**. These MPCs and NCs are scientifically-derived risk limits based on the premises

formulated by the government with respect to the desired level of protection of human beings and ecosystems.

For substances with a clear concentration level below which there are no effects (threshold level), the MPC for human beings is set to the no-effect level for man (NOEL). Very often this NOEL is extrapolated from the no-effect level that is found in chronic laboratory studies with test animals. However, in some cases the basis for the final MPC can also comprise epidemiological information.

Substances without a clear threshold below which there are no effects (e.g. carcinogens) can still cause adverse effects, even at very low concentrations. For these substances the concentration at which there is annually 1 death per 1 million people (risk 10^{-6} /year) is set as the MPC.

The MPC should in principle also protect ecosystems. The policy of safeguarding ecosystems against pollutants is based on protecting both the structure (the species) and functions of ecosystems. For aquatic and terrestrial ecosystems it is assumed that protecting the structure (the qualitative and quantitative distribution of species) will also safeguard the functional characteristics of the system. However, our knowledge on the effects of substances on ecosystems is limited and different extrapolation techniques have to be applied to derive the no-effect concentrations for ecosystems from single species laboratory toxicity data. In case there is limited information available, fixed assessment factors are applied to the lowest acute or chronic toxicity concentrations found in laboratory experiments. In case there is a larger amount of chronic toxicological information available a statistic extrapolation model, taking into account differences in sensitivity between species, is used to derive the MPC for ecosystems. As the relationship in the model between the concentration and percentage of protected species is asymptotic, a limit for the protection percentage had to be chosen to derive realistic concentration values. This value is set at 95%, assuming thereby to protect the whole ecosystem.

The MPC is set per individual compound. However, in the environment man as well as ecosystems are exposed in an uncontrolled manner to many unknown substances coming from one and the same source or from a variety of sources. The consequences of the resulting cumulative exposure in terms of an accumulation of effects are unknown. Since environmental policy seeks to achieve a no-risk level at the longer term, a greater margin of safety is needed to account for combined exposure to a large number of threshold value substances. Therefore the NC-risk limit is formulated which in principle is set at 1 % of the MPC for each individual substance. Although no scientific basis can be provided for this safety factor 100, the need for this approach is underlined by the fact that it has been demonstrated in aquatic ecosystems that, as a result of additivity, effects may still occur at concentrations lower than the MPC for individual substances.

For substances without a threshold, generally carcinogenic substances, the NC for humans is based on the existing international consensus that a risk of tumour formation of 1 in 100 million annually (risk 10^{-8} /year) can be considered negligible.

1.2 Harmonisation of risk limits

For historical reasons quality standards were developed firstly for food, drinking water, the workplace area and for outdoor air. Hence, these standards were strongly human-oriented and mainly based on mammalian toxicological information. Since the beginning of the eighties, the protection of the environment by

protecting ecosystems has gained more attention and calculation of no-effect concentrations for the environment has now become a standard procedure in several countries. At present, most environmental quality standards are being set in a way that both man and ecosystems are protected by direct as well as indirect exposure routes.

Despite these recent developments the effect-oriented environmental policy in most countries is still characterised by a compartmental approach. Environmental quality standards are determined for the compartments air, water and soil separately, not taking into account the transport of chemicals from one compartment to another due to (natural) physico-chemical processes (atmospheric deposition, sedimentation, volatilisation). Therefore effects can be caused in organisms in other compartments than those to which the chemicals have been released. Thus, harmonisation of these standards is highly necessary because of the fact that (1) releases of chemicals to water and soil can, after volatilisation, lead to deleterious effects in the air, either to man or to parts of the ecosystems and (2) because air and water can be important transport media for many chemicals which may affect the quality of water, sediment and soil. Hence, achieving concentrations lower than the quality standard for one compartment does not necessarily mean that a 'safe' concentration in another compartment can be obtained and maintained.

Based on this observation a few years ago in the Netherlands a project entitled 'Setting Integrated Environmental Quality Standards' was started. The aim of this project was the development of a set of environmental quality standards for air, water and soil that are set in such a way that they meet a coherence-criterion. This coherence-criterion implies that standards for one compartment have to be set at a level where protection to organisms living in other compartments is ensured as well.

1.3 Application of risk limits in environmental policy

The scientifically-derived risk limits presented in this document are the basis for non legally binding environmental quality standards that are applied in environmental policy in The Netherlands. In the Third National Environmental Policy Plan (NEPP, 1998) a definition has been given for the environmental quality standards used in the Dutch Environmental Policy. The MPC is, as mentioned previously, a scientifically-derived value for a compound, indicating the concentration where either no effect can be expected or (for compounds without a threshold value) a risk of 10⁻⁶/year is accepted.

The target value is defined as the value indicating when the adverse effects caused by a certain compound can be considered as negligible. In most cases the target value is set at the NC.

For naturally occurring chemicals, such as metals, a special approach has been followed based on the assumptions that effects on biota caused by ambient background concentrations of metals are not considered as adverse effects, in respect of evaluating source abatement policy. Therefore it is decided to define the MPCs of metals as the sum of a risk concentration and the ambient background concentration in The Netherlands. The target value for metals is set at the sum of NC and ambient background concentration.

In the NEPP3 (NEPP, 1998) the MPC has been set as a short term target, which must no longer be exceeded by the year 2000 as a result of emissions. The target value can be seen as the long-term target for environmental policy, if possible to be achieved by 2010. In between these two risk limits there is a so-called grey

area where reduction of the risks is preferable according to the ALARA principle (as low as reasonable achievable).

As mentioned previously environmental quality standards are policy instruments that in practice can be used for a number of applications in environmental policy.

The applications of MPCs and target values are formulated in the NEPP3 (NEPP, 1998) as follows:

1. Assessment of the environmental quality of a specific area or site.

Evaluation of the quality of a certain site (water, soil, sediment or air) is probably the field where quality standards are applied most frequently. Here, quality standards help in judging whether or not there may be risks to man and/or the ecosystems by comparing the environmental concentration of the chemical with its environmental quality standard. The MPCs and target values for water and sediment and its applications are published in the Fourth Policy Document on Water Management (1998). For soil intervention values and the target values are used as environmental quality standards (Circular on intervention and target values-soil quality standards-, 1994).

2. Underpinning of source-oriented emission abatement strategies, especially priority setting

Based on the exceedance of environmental quality standards a prioritisation can be made in which area emission reduction measures should be carried out first. As mentioned previously, environmental quality standards can be applied in order to evaluate the effectiveness of the emission reduction policies (monitoring, see also 5).

3. Assessment of future legislation of environmental quality guidelines/standards

The MPCs and target values are usually published in environmental policy documents and/or plans. This means in effect that they are not legally binding to other authorities. Assessment of environmental quality by using MPCs and/or target values might give rise to develop legally binding standards for compounds of concern.

4. Standards for products- and pesticides policy.

In The Netherlands the MPCs used for decisions whether or not pesticides are admitted for application are identical to the MPCs used for environmental quality assessments and related policies.

5. Evaluation and formulation of national policy standards on emission reduction.

In case the environmental quality standard for a specific substance is exceeded, due to multiple point and diffuse sources (national as well as international), it may be useful to indicate to what extent emissions of these sources should be reduced in order to meet the environmental quality standards. These emission reduction percentages are now subject of negotiations with the target groups using the ALARA principle in order to get agreement about the emission reductions to achieve the targets for 2000 and 2010 .

6. Granting permits.

The government and other licensing authorities have to decide whether or not permits for emissions are to be granted. According to the Pollution of Surface Waters Act one of the aspects which plays a role in such a decision is the influence of the emission of concern on the environmental quality of the receiving

waters.

The present document is restricted to a survey of the MPCs and NCs that are scientifically-proposed by RIVM and gives a description of the procedures that are used to derive them. In addition, all the relevant underlying data that have been used are listed. The environmental quality standards used in Dutch environmental policy are listed in the enclosed policy document 'Setting Integrated Environmental Quality Standards: Environmental quality standards for soil, water & air, 1999'. In principle the scientifically-proposed MPCs and NCs are directly set as MPCs and target values for Dutch environmental policy. However, if another number was set than the scientifically-proposed MPC or NC it is explained in the enclosed policy document.

Consultation

The risk limits presented in this document have all been discussed in the advisory group of the project 'Setting integrated environmental quality standards'. In this advisory group experts from various governmental research institutes participate. Subsequently, the National Health Council of The Netherlands and the Technical Soil Protection Committee have reviewed the derivation methods and proposals for MPC and NC values published in the reports of the National Institute of Public Health and the Environment (RIVM) as is described in Chapter 2. The comments of these advisory boards have been taken into account as much as possible for the final derivation of risk limits and setting of environmental quality standards.

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2. PROCEDURE TO DERIVE MAXIMUM PERMISSIBLE CONCENTRATIONS

2.1 General introduction

Maximum permissible concentrations (MPCs) are derived for every individual compartment, air, water, sediment and soil according to the risk philosophy as described in Chapter 1. In principle, these MPC values should protect man as well as ecosystems. Hence, where possible, information on the toxicological and ecotoxicological effects of a chemical is taken into account. For most compounds the assumptions have been made that organisms in ecosystems are probably more exposed to those compounds in water, sediment and soil than humans. Therefore, the MPC values are usually based on ecotoxicological data. Since human beings are more directly exposed to compounds via air, for instance for volatile compounds, the MPC for this compartment is derived from mammalian inhalation studies or, if available, from epidemiological studies. In addition, a first attempt is made to take into account the ecotoxicological effects on organisms that are mainly exposed to air. However, those data to perform such an assessment are usually lacking.

The procedure to derive an MPC for water, sediment, soil and air, based on ecotoxicological data, is described in section 2.2 of the present chapter. Section 2.3 describes the procedure to derive an MPC for air based on toxicological data.

Figure 1 provides a flow diagram of the different steps leading to integrated environmental quality standards. The process starts with the collection of toxicological and ecotoxicological data and data on physico-chemical properties. Toxicity data are selected which meet certain quality criteria and are subsequently treated according to specific procedures to make them applicable as input for the extrapolation methods that are used to derive MPC and NC values for the different compartments. The procedures and quality criteria that are applied are summarized in Annex 1. The procedure to derive MPCs for air, soil, sediment and water is explained in the present chapter. The next step in the procedure is the harmonization of the MPCs and NCs for the different compartments. This is explained in Chapter 3. Finally, setting of target and/or limit values based on the harmonized MPCs and NCs can take place. This process is not explained further in detail in this document.

Figure 1: General procedure to derive harmonized environmental quality standards (EQSs).

2.2 Derivation of MPCs based on ecotoxicological effects data

2.2.1 Introduction

The general approach in the ecotoxicological effect assessment is schematically presented in Figure 1. Depending on the information available, different extrapolation methods are used to estimate a maximum permissible concentration (MPC) for the ecosystems. A refined and a preliminary effect assessment method can be distinguished. When (sub)chronic data on effects of a substance on survival, reproduction, growth or photosynthesis for four or more taxonomic groups are available a refined effect assessment method can be used. This method will be explained in § 2.2.2.2. If less information is available on the ecotoxicity of a compound a preliminary effect assessment method is used to derive an MPC (see § 2.2.2.1).

If laboratory toxicity data are insufficient or lacking, the toxicity data can be obtained using Quantitative Structure-Activity Relationships (QSARs). QSARs are based on the relation between the physico-chemical properties of a compound and ecotoxicological criteria such as L(E)C₅₀ or NOECs. These estimated

toxicity data can be used in the above mentioned refined and preliminary effects assessment methods. In § 2.2.3 this QSAR approach will be explained.

The preliminary and refined effects assessment methods also apply to soil or sediment. However, since the toxicity data for soil or benthic organisms are often lacking alternative methods will have to be used. Therefore, the MPC_{soil} or the $MPC_{sediment}$ of a compound may be derived from the MPC for aquatic organisms based on the concept of equilibrium partitioning (EP). This EP-method will be explained in § 2.2.4.

Figure 2: Schematic presentation of ecotoxicological effect assessment of substances

The methods for ecotoxicological effects assessment as described above do not account for indirect effects of chemicals. Animals that prey on aquatic organisms containing high levels of (mainly persistent) contaminants may take up a considerable amount of the chemical by their food. Hence, exposure to contaminated food may lead to secondary poisoning of species at the top of the food chain, for instance along the pathway water→fish→fish-eating bird or mammal. Secondary poisoning is a typical phenomenon for compounds with a high potential for bioaccumulation such as highly hydrophobic substances ($\log K_{ow} > 3$) and some metal-compounds. The methodology to take possible effects of secondary poisoning into account in standard setting is described in § 2.2.5.

Ideally, the effects of a chemical should be tested in a natural system representative of an area that is to be protected. In test systems with a higher level of complexity ranging from multi-species laboratory systems to microcosms, outdoor ponds, enclosures and field trials, effects are studied under variable environmental conditions and include population dynamics, interactions between species, and between species and the abiotic environment. The data derived from field (multi-species) studies will be used as additional information for the derivation of an ecotoxicological MPC. However, usually these data are scarce. Furthermore, studies in more complex systems are not only difficult to perform and expensive in terms of time and money, they are also difficult to interpret, among others from a statistical point of view.

Compounds that occur naturally in the environment, such as metals, are treated differently from organic substances. Firstly, some metals are essential to organisms, specific attention needs to be paid to the quality of the toxicity test in terms of breeding conditions and availability of the necessary elements. Secondly, since for some metals relatively high natural background concentrations are found in the environment, these background concentrations need to be evaluated and taken into account in setting the risk limits. This methodology is described in § 2.2.2.3.

The MPC and NC values for surface water apply in principle to dissolved concentrations (i.e. concentrations in the water after filtration through a 0.45 µm filter), and not to suspended matter. If risk limits for total concentrations are needed the dissolved concentrations need to be corrected to take into account the fraction of the substance that is adsorbed to the suspended matter (using a standard suspended matter concentration of 30 mg/l). For soil and sediment the MPC and NC values apply to so-called 'standard soil' with fixed characteristics (10 mg/kg organic matter and 25 mg/kg clay). For soils and sediments with different characteristics these MPC values need to be corrected using specific normalization procedures. These procedures are similar to the procedures that are applied to normalize toxicity data, as described in § 2.1 of Annex 1.

2.2.2 The extrapolation methods

For the estimation of a 'safe' level below which no adverse effects in the environment are expected to occur, usually an extrapolation factor has to be applied to the available toxicity data. Ideally, this extrapolation factor should account for:

- interspecies variation in sensitivity;
- acute to chronic toxicity extrapolation;
- laboratory data to field impact extrapolation.

Various methods have been proposed to extrapolate from single-species toxicity data to a concentration which protects the ecosystems (OECD, 1992^a). In The Netherlands two extrapolation methods are used to estimate an MPC for the ecosystems, depending on the availability of toxicity data: 1) the preliminary effect assessment method that applies fixed assessment factors to the lowest available toxicity data, and 2) the refined effect assessment method that uses statistical extrapolation techniques.

The risk philosophy, regarding the safeguarding of ecosystems, is based on the protection of both the structure (the species) and functions of ecosystems. For aquatic and terrestrial ecosystems, it is assumed that protecting the structure (the qualitative and quantitative distribution of species) will also safeguard the functional characteristics of the system, e.g. respiration, ammonification, mineralization for soil ecosystems. Because this assumption is theoretically debatable (Slooff, 1992), information that is not specifically species-related but related to the functioning of a group of species is also used in the effect assessment. In order to use the information about effects on structural and functional parameters as input data for extrapolation methods, the data must be expressed as $L(E)C_{50}$ s or NOECs. In the refined effect assessment method, the data on structural and functional parameters are treated separately, while in the preliminary effect assessment method no distinction is made between these data.

In the extrapolation methods used only one value per species is used as input. If more than one value for a certain species or process is available, one value is selected or calculated for use in the extrapolation.

When selecting data the following rules are applied (Slooff, 1992):

- Toxicological criteria which may affect the species at the population level are taken into account. In general these are survival, growth and reproduction and are commonly expressed as an $L(E)C_{50}$ (short-term tests, duration four days or less) or NOEC (long-term tests, duration more than four days, with the exception of microorganisms and algae for which a NOEC may be derived from experiments during less than four days).
- If for one species several toxicity data based on the same toxicological endpoint are available, these values are averaged by calculating the geometric mean.
- 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 (see above).
- In some cases data for effects of different life-stages are available. If from these data it becomes evident that a distinct life-stage is more sensitive, this result may be used in the extrapolation.

For soil, toxicity data on terrestrial species as well as for microbial and enzymatic processes may be available. The latter are in principle summed parameters expressing the performance of a process. The process in question may be performed by more than one species and under toxic stress, the functioning of the process may be taken over by less sensitive species. From the foregoing it may be clear that effects on species and effects on processes are quite different. According to Van Beelen and Doelman (1996) the results of ecotoxicological tests with microbial processes cannot be used in combination with single-species tests in one extrapolation, because of the differences between them. Therefore, these data are not combined and individual values are derived.

For the data on microbial and enzymatic processes more than one value per process is included in the extrapolation method. It is reasoned that NOECs for the same process but using a different soil as substrate are 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 value is selected or calculated.

2.2.2.1 The preliminary effect assessment method

The preliminary effect assessment method is applied when less than four chronic NOECs are available from different taxonomic groups. With this method fixed assessment factors are applied to the lowest value in the available data set. This method, also called the modified EPA method, estimates an MPC (OECD, 1992^a). The empirically derived assessment factors are not based on any theoretical model, but have been developed in line with experience with chemical effects assessment. The assumption is made that there is a constant and identical difference between acute and chronic toxicity and between single-species (laboratory) and ecosystem sensitivity. Hence, the assessment factors may be used to extrapolate from the lowest chronic NOEC to the field situation and from concentrations with acute effects to no-observed effect concentrations (EPA, 1984). For each extrapolation step a factor 10 is suggested. Compared to the refined effect assessment method the modified EPA method is relatively straightforward. It has the advantage that it can be applied if only one acute or chronic test result or even one QSAR-estimate of toxicity is available.

Surface water

The modified EPA method was originally developed for the compartment surface water, and is internationally accepted (OECD, 1992^b). The information on aquatic toxicity data and the subsequent assessment factors are presented in Table 1.

Table 1: The assessment factors of the modified EPA method for aquatic species (water)

Available information	Assessment factor
Lowest L(E)C ₅₀ value or QSAR estimate for acute toxicity	1,000
Lowest L(E)C ₅₀ value or QSAR estimate for minimal three representatives of algae/crustaceans/fish	100
Lowest NOEC value or QSAR estimate for chronic toxicity for minimal three representatives of algae/crustaceans/fish	10
Lowest NOEC value for chronic toxicity	10*

* This value is subsequently compared to the MPC based on acute L(E)C₅₀s. The lowest one is selected.

If chronic data or reliable QSAR estimates for chronic toxicity for the three taxonomic groups mentioned in the table (algae, crustaceans and fish) are available, an assessment factor of 10 is used on the lowest NOEC of the data set. This extrapolated value will be used as the MPC in surface water. If NOECs for less than three mentioned taxonomic groups are available, also an assessment factor of 10 is applied to the lowest NOEC. This value will subsequently be compared to the extrapolated value based on L(E)C₅₀s. The lowest value is selected as the MPC.

If, for example for a substance an LC₅₀ of 100 µg/l for crustaceans and a NOEC of 50 µg/l for fish are available, the extrapolated value based on the LC₅₀ will be

$100/1000 = 0.1 \mu\text{g/l}$, and the extrapolated value based on the NOEC will be $50/10 = 5 \mu\text{g/l}$. Hence, the MPC in surface water is $0.1 \mu\text{g/l}$ (the lowest value).

Soil

A similar approach as with surface water is applied to extrapolate laboratory toxicity data on soil organisms to an MPC for soil (Table 2). Analogously to the procedure for surface water, assessment factors depend on the type of investigations (acute or chronic), the number of trophic levels as well as the general uncertainties in predicting ecosystem effects from laboratory data. It should be noted that this method is not yet internationally accepted. Especially the choice of taxonomic groups for which toxicity data are required, is still a point of discussion.

Table 2: The assessment factors of the modified EPA method for terrestrial species (soil)

Available information	Assessment factor
Lowest L(E)C ₅₀ value for acute toxicity	1,000
Lowest L(E)C ₅₀ value for minimal three representatives of microbial mediated processes, earthworms and arthropods or plants	100
Lowest chronic NOEC for minimal three representatives of microbial mediated processes, earthworms and arthropods or plants	10
Lowest NOEC value for chronic toxicity	10*

* This value is subsequently compared to the MPC based on acute L(E)C₅₀s. The lowest one is selected.

If chronic data or reliable QSAR estimates for chronic toxicity for the taxonomic groups mentioned in the table are available, an assessment factor of 10 is used on the lowest NOEC of the data set. This extrapolated value will be used as the MPC in soil. If NOECs for less than three mentioned taxonomic groups are available, also an assessment factor of 10 is applied to the lowest NOEC. This value will subsequently be compared to the extrapolated value based on L(E)C₅₀s. The lowest value is selected as the MPC.

Air

As mentioned in section 2.1 at the moment there is very little information available on the possible ecotoxicological effects of chemicals on organisms from exposure through air. Since the data are lacking, there is a large uncertainty in the selection of test species as well as in the assessment factors that must be applied. Slooff and Tingey (1991) were the first to propose the modified EPA method to air at 'The 3rd US-Dutch expert workshop on comparative risk analysis for air pollution prevention' in 1991. Slooff and Tingey (1991) suggested mammals, birds, plants or lichens, and insects as representative taxonomic groups for the part of the terrestrial ecosystems exposed to air pollutants. Based on the modified EPA method, assessment factors in relation to the availability of data for these taxonomic groups were proposed. These factors are given in Table 3. When the relevant information is available, this method is used to obtain an indication what the no-effect levels for the ecosystems are. It is currently not used to set MPC values for air.

Table 3: The assessment factors of the modified EPA method for mammals and birds (air)

Available information	Assessment factor
Lowest L(E)C ₅₀ value for acute toxicity	1,000
Lowest L(E)C ₅₀ for minimal three representatives of mammals or birds, plants or lichens, and insects	100
Lowest NOEC for minimal three representatives of mammals or birds, plants or lichens, and insects**	10
Lowest NOEC value for chronic toxicity	10*

* This value is subsequently compared to the extrapolated value based on acute L(E)C₅₀s. The lowest one is selected.

** Sub-acute data on birds and mammals (< 1 month) are extrapolated to chronic data by applying an extra factor of 10.

2.2.2.2 The refined effect assessment method

The refined assessment method is applied when sufficient ecotoxicological data are available, i.e. chronic NOECs from four or more different taxonomic groups. The refined assessment method of Aldenberg and Slob (1993) assumes that the NOEC values used for estimating the distribution fit a log-logistic distribution. If the NOECs are not log-logistically distributed and some of the data cannot be rejected for specific reasons, the refined as well as the preliminary effect assessment methods are applied and the results are compared. The lowest value is considered as the MPC.

The aim of environmental quality standards is that the MPC is set at a level that protects all species in an ecosystem, i.e. not only fish, *Daphnia* or algae. However, in order to be able to use extrapolation methods such as that of Aldenberg and Slob (1993), a cut-off value is set at 5% (Fraction of species unprotected: $F_u = 0.05$; or the Hazardous Concentration for 5% of the species: HC5), i.e. a 95% protection level is chosen at the cut-off value (VROM, 1989). The concentration corresponding to a 95% protection level is called the MPC, can be derived using statistical extrapolation methods, and as stated earlier, is assumed to protect all ecosystems.

Statistical extrapolation methods are based on the assumption that the sensitivities of species in an ecosystem, expressed as NOEC or L(E)C₅₀ values, can be described by a statistical frequency distribution. This frequency distribution can be estimated using NOEC or L(E)C₅₀ values of species of different taxonomic groups as input. From the estimated distribution a concentration can be derived which is assumed to be "safe" for an ecosystem. 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).

The method of Aldenberg and Slob (1993) is used in the project "Setting Integrated Environmental Quality Standards" if NOEC values for four or more different taxonomic groups are available. This method assumes that the NOEC values used for estimating the distribution fit the log-logistic distribution. For checking this assumption the available data can be tested statistically with the empirical distribution function (EDF): Kolmogorov-Smirnov $D \cdot \sqrt{n}$ test

(Aldenberg and Slob, 1993). If the distribution of NOECs is rejected at a significance level of 1% it is unlikely that the NOECs are log-logistically distributed. This may occur with chemicals that have a very specific mode of action. The advantage of the log-logistic distribution is that it allows the analytical evaluation of the cumulative distribution $F_u(x)$ by integration:

$$F_u(x) = \frac{1}{(1 + \exp(\frac{\alpha - x}{\beta}))} \quad (1)$$

in which:

- $F_u(x)$ = fraction of species unprotected at concentration x
- α = mean value of the log-logistic distribution
- β = scale parameter of the log-logistic distribution
- x = $\log(c)$: logarithm of the concentration

The log-logistic distribution can be characterised by α and β . The α indicates the mean value of the distribution which determines the location of the distribution on the concentration axis ($\log(\text{NOEC})$ or $\log(c)$) and β is the scale parameter of the distribution which determines the width or shape of the distribution and is equal to approximately half times α ($\beta = \sigma \cdot \sqrt{3/\pi}$). In Figure 3 some examples of the log-logistic frequency distribution and in Figure 4 of the cumulative log-logistic distribution are shown.

$F_u(x)$ has a value between 0 and 1 and is the fraction of species that have $\log(\text{NOEC})$ values smaller than x . When F_u is equal to 0.05, the corresponding concentration can be calculated with 50% and 95% confidence. In The Netherlands the MPC is set equal to the former value. The concentration, corresponding to a certain fraction of species unprotected can be derived by rewriting equation 1 into:

$$x = \alpha - \beta \ln \{(1 - F_u)/F_u\} \quad (2)$$

Figure 3: Examples of log-logistic frequency distributions with different α and β values

Figure 4: Examples of cumulative log-logistic distributions with different α and β values (see also equations 1 and 2)

The Negligible Concentration (NC), in contrast to the MPC, is not based on a fraction of species protected and is derived by dividing the MPC by a factor 100. This factor is applied to take combination toxicity.

2.2.2.3 The added risk approach

Some substances, such as metals, have natural sources. In addition, some metals are essential for life and have natural background concentrations. Organisms require a certain amount of these essential elements, but experience toxic effects when exposed to too high concentrations. The natural background concentrations of those metals are thus essential and result among others in the biological diversity of ecosystems. While naturally-occurring chemicals may thus also impose a stress, it is common practice to refer to their impact as 'effects', rather than 'adverse effects'. Nevertheless, such effects can be similarly quantified as F_u , the fraction unprotected.

For some metals the MPC and/or NC values that are calculated according to the procedures described in the previous sections can be lower than the background concentration. Until recently, the environmental quality standards (EQSs) were set on this background concentration level. As a result these EQSs were not based on risk considerations and when comparing the EQS with actual concentrations it was not possible to assess the risk of these actual concentrations.

Recently, a method called 'the added risk approach' was proposed by Struijs et al. (1997). With this method it is possible to quantify the risk of a naturally occurring substance, such as metals, as the maximum fraction of all possible species ($F_{u_{max}}$) that is unprotected, due to an active concentration of that naturally-occurring substance considered. In this $F_{u_{max}}$, effects of both the background and of the anthropogenic concentration added to this, are included. An extensive description of this method can be found in Struijs et al. (1997).

For metals and other naturally-occurring substances, the Maximum Permissible Addition (MPA) is thus defined as the concentration that may be added on top of the background concentration. The basic starting point for this approach is the calculation of the Maximum Permissible Addition (MPA) that is calculated on the basis of the available data from laboratory toxicity tests. This MPA, which is assigned to anthropogenic activities, is subsequently added to the background concentration (Cb) of the substance leading to the Maximum Permissible Concentration (MPC). In formula:

$$MPC = MPA + Cb \quad (3)$$

Whether or not the background concentration is bioavailable or may even lead to deleterious effects on the ecosystem is ignored, since from an environmental policy point of view these effects can be regarded as desirable since they may lead to an increase in biodiversity. Although from a policy point of view those effects due to the actual bioavailable fraction and deleterious effects may be ignored, a more scientific investigation of the resulting outcome of the approach as published by Struijs et al. (1997) may, however, be warranted, as is earlier discussed by Struijs et al. (1997).

The existing statistical extrapolation methods are elaborated into the "added risk approach" to be used for all substances naturally-occurring or anthropogenic, with which the MPA can be calculated.

The added risk approach as published by Struijs et al. (1997) is followed in the present report, but it must be mentioned that the terminology as proposed by Struijs et al. (1997) has been slightly modified. Whereas Struijs et al. (1997) assume that the background concentration consists of an active or bioavailable fraction and an inactive or not bioavailable fraction, the present report assumes that the background concentration is not relevant for the risk limits. With regard to the bioavailable fraction of the metals in laboratory tests, it is assumed that the added metals to the test medium is completely bioavailable, i.e. the bioavailable fraction of the added metal in the laboratory tests is 100%.

The Negligible Addition (NA) is obtained by dividing the MPA by 100:

$$NA = \frac{MPA}{100} \quad (4)$$

The NC is obtained by adding NA and the background concentration to:

$$NC = NA + Cb \quad (5)$$

After an extensive discussion on the application of the added risk approach for the metals that are dealt with in this report it was concluded that (for details see the enclosed report of Crommentuijn et al. (1997a)):

- For some metals the background concentration is very low compared to the ecotoxicological effects data. This situation is comparable with the situation for xenobiotics which have a background of zero and the procedure reduces to the Aldenberg and Slob method as described in § 2.2.2.2.
- For some metals there is a significant background concentration compared to the ecotoxicological effects data. It was decided to exclude the background concentration for deriving risk limits, which thus implies that the MPA is set at the HC5. Therefore, the background concentration is not included in deriving the MPA, but is included in deriving the MPC (since: $MPC = MPA + C_b$).

Although in both situations the calculation procedure reduces to the Aldenberg and Slob method, application of the added risk approach for risk assessment of metals implies that the MPA and the background concentration need to be summed. Therefore, in Part II 'Risk Limits' of this document both the background concentration and the MPC and NC values will be given for every metal.

2.2.3 QSAR approach

Usually data from single-species tests are used to predict effects in the environment. For some chemicals these single-species toxicity data are not available. This lack of information on ecotoxicological effects urged the need to develop a more pragmatic approach, by which a reliable estimation of the toxicity (LC_{50} or NOEC) of an environmental pollutant can be made. This pragmatic method uses Quantitative Structure-Activity Relationships (QSARs) to estimate single-species toxicity data. 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. Recently six modes of action were 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. An additional advantage is that QSARs are available for more species than the species for which toxicity data from literature are usually available.

For narcosis type chemicals, QSARs are available for a large number of species. Estimated chronic toxicity data can be used as input in extrapolation models. Van Leeuwen et al. (1992) selected 19 QSARs, comprising species of different trophic levels and taxonomic groups from the literature. These QSARs are used to derive an estimation of the semi-chronic toxicity for aquatic organisms. The QSARs, expressed as $\log \text{NOEC} = a \log K_{ow} + b$, are presented in Appendix 4. By filling in the $\log K_{ow}$ of a substance, 19 estimated NOECs can be derived. These NOECs are subsequently used to calculate an HC5 under the assumption of a log-logistic distribution according to Aldenberg & Slob (1993). HC5-values are presented in Appendix 4.

2.2.4 Derivation of MPC values for sediment and soil with the Equilibrium Partitioning method (EP-method)

Sediments may act as a sink for, and source of chemicals through sorption of chemical contaminants to particulate matter. Sediments integrate the effects of surface water contamination over time and space, and may thus present a hazard to aquatic communities (both pelagic and benthic) which is not directly predictable from concentrations in the water column. Effects on benthic organisms are of concern because in many habitats the sediment plays an important role in the recycling of detrital material. Therefore, sediment quality standards should be derived that may serve as a basis for standards to protect benthic organisms and the aquatic system from the effects of sediment contamination.

A large number of different methods is available to derive sediment quality standards, all with specific advantages and limitations (OECD, 1992^b). In the absence of any ecotoxicity data on soil or benthic organisms a relatively simple approach to derive sediment or soil risk limits is the so-called Equilibrium Partitioning (EP) method (Shea, 1988). The method assumes a sorption equilibrium between the concentrations in water and in the sediment. The method is applicable to chemicals for which a partitioning model, describing the sediment partitioning as a function of the properties of the chemical and the characteristics of the sediment, is available. The method is based upon the observation that the toxicity of the chemicals in sediments to benthic organisms is related more closely to the concentrations in interstitial water than to the bulk sediment concentrations. Following the outcome of an international OECD workshop (OECD, 1992^b), the EP-method relates - by assuming steady-state - the concentration in sediment to a concentration in (interstitial) water. Consequently an MPC for (interstitial) water can be converted to an MPC for sediment assuming that:

- The concentrations in sediments, interstitial water, and benthic organisms are at equilibrium.
- The concentration of a chemical substance in any of these phases can be predicted using appropriate partition coefficients and concentrations in one phase.
- Concentrations in sediments causing effects, expressed on the basis of the organic carbon content, can be predicted using partitioning predictions and effect concentrations in water.
- The water risk limit criterion is an appropriate effects concentration for deriving sediment quality standards.
- Species living in sediment are mainly exposed through the water phase.

Sediment

Based on the above mentioned assumptions the MPC in surface water can be used to predict the MPC in sediment as follows:

$$MPC_{\text{sediment}} = K_p \cdot MPC_{\text{surface water}} \quad (6)$$

with:

MPC_{sediment}	=	MPC for bulk sediment (in mg/kg)
$K_{p_sediment}$	=	sediment/water partition coefficient (l/kg) (see Annex 1, § 4.2);
$MPC_{\text{surface water}}$	=	MPC in surface water based on ecotoxicity data on aquatic organisms (in mg/l).

For substances for which the "added risk approach" is used, the MPC for soil or sediment is derived from the MPA for water as a starting-point and to which the background concentration for soil or sediment is added. Analogously, the NC is derived by dividing the MPA by 100 and adding the background concentration: $NC = (MPA/100) + C_b$ (see equation 5).

The processes that govern the partitioning of chemicals among sediment, interstitial water and biota are better understood for non-polar organic substances than for other chemicals. For non-polar organic chemicals the concentration ratio between sediment and interstitial water is strongly determined by the organic carbon fraction in the sediment phase. Hence, normalisation for the organic carbon content of the sediment provides a means to make the sediment quality standards applicable to a wide range of sediments. The normalisation procedure is described in § 2.1 of Annex 1.

The first assumption about the equilibrium situation is that it is applicable to neutral organic chemicals, but not to highly polar and charged organic compounds and for compounds which are rapidly degradable, for which it is not possible to model sorption in such a simple manner as for neutral organic chemicals (Van der Kooy et al., 1991). In addition, with respect to the assumption that soil and benthic organisms are exposed only via interstitial water, it should be noticed that this is probably not valid for highly hydrophobic compounds for which uptake by food or sediment cannot be excluded (Van der Kooy et al., 1991; Belfroid et al., 1996).

The approach for metals is essentially the same, but in this case, values of K_p are to be derived from the results of routine surveys of the water quality. It should be noted that K_p values for metals show a great variability and depend on many physico-chemical factors such as salinity, pH, dissolved oxygen concentration (Bockting et al., 1993). In addition, it must be noted that the toxicity of divalent metals in sediment is probably related to the level of acid volatile sulphide (AVS) in the sediment phase (DiToro et al., 1990). Adverse effects on benthic organisms will likely occur only when the ratio of the metal to the AVS content (both expressed in $\mu\text{mol/g}$) exceeds unity. Therefore, AVS appears to provide a better method for normalisation of sediments with different metals contents and may lead to a different approach to set sediment risk limits in the future. At present, only limited information is available on the AVS content in Dutch sediments (Van den Hoop et al., 1995).

Soil

In case there are too few terrestrial toxicity data available to use the methods described in section 2.2.2, the EP-method is applied to derive an MPC in soil. It should be noted, however, that the method has been tested less for soil organisms than for benthic organisms. As with sediment, the assumption is made that the toxicity of chemicals for soil organisms is principally determined by the concentration in the interstitial water. This concept was extensively studied by Van Gestel and Ma (1993) who showed that the toxicity of several chlorophenols, chlorobenzenes and chloroanilines for earthworms is predominantly correlated to interstitial water concentrations.

The formula used to calculate an MPC in soil is as follows:

$$MPC_{soil} = K_p \cdot MPC_{surface\ water} \quad (7)$$

with:

MPC_{soil}	=	MPC in bulk soil (in mg/kg)
K_{p_soil}	=	soil/water partition coefficient (l/kg) (see Annex 1, § 4.2)
$MPC_{surface\ water}$	=	MPC in surface water based on toxicity data on aquatic organisms (in mg/l).

2.2.5 Secondary poisoning

By applying the methods described so far, MPCs are determined taking into account direct effects on organisms living in the environment. However, direct exposure to a compound can lead to accumulation in organisms which may result in deleterious indirect effects in higher members of the food chain (top predators). This is called "secondary poisoning" which will mainly occur with organic compounds with a relatively high hydrophobicity ($\log K_{ow} > 3$) and a molecular weight of less than 600 g/mol and with some metals. A methodology has been developed to include effects due to secondary poisoning in the derivation of MPCs (Romijn et al., 1993). The basic assumption of that method is that a concentration in the food of top-predators can be determined at which no adverse effects occur. The concentration in the food is directly related to the concentration in the environment through bioconcentration and bioaccumulation. Hence, it is in principle possible to translate the no-effect concentration (NEC) in the food, to a no-effect concentration in the media (surface water or soil) to which the prey of the top-predators are exposed, if the appropriate toxicity and bioaccumulation data are available.

At the moment three possible food chains are distinguished through which top predators can possibly be exposed to hazardous compounds: for the aquatic environment: water → fish → fish-eating bird or mammal (Romijn et al., 1993), and water → mussel → mussel-eating bird or mammal (Jonkers and Everts, 1992), and for the terrestrial environment: soil → worm → worm-eating bird or mammal (Romijn et al., 1994). Although the approach for the aquatic food chains is considered better applicable than for the terrestrial food chain (National Health Council, 1993), both food chains are included in deriving risk limits for secondary poisoning.

The following formulas are used to calculate an MPC for secondary poisoning for the aquatic and the terrestrial route, respectively:

water:
$$MPC_{sec, pois.} = NEC_{predators} \frac{CF}{BCF_{fish/mussel}} \quad (8)$$

soil:
$$MPC_{sec, pois.} = NEC_{predators} \frac{CF}{BCF_{earthworm}} \quad (9)$$

with:

- $NEC_{predators}$ = No Effect Concentration (NEC) for predators derived from extrapolations of results from dietary laboratory toxicity test with animals representative for predators (in mg/kg food)
- CF = correction factor for the caloric content of food in the laboratory versus the field situation
- BCF = bioconcentration factor (in l/kg).

The derivation of the NEC for predators, the determination of bioconcentration factors and the correction factors for the caloric content of food will be described in the following paragraphs.

Derivation of the NEC for predators

In order to derive a NEC for predators ideally long-term toxicity data have to be available for these organisms. However, laboratory experiments with predators are rare: for mammals and birds most laboratory toxicity tests have been carried out on species such as rats, mice, hens, pheasants and quails. So, dietary studies with these organisms are used and considered to be representative for predators. The selected L(E)C₅₀s and NOECs for birds and mammals have to be extrapolated to derive a NEC for predators. When more than four NOEC values are available the refined effect assessment method is used for the derivation of the NEC (see section 2.2.2.2). In this case, long term NOEC values for individual species are used as input data. In case only few data are available, a preliminary effect assessment method is used. The assessment factors for this method are presented in Table 4.

Table 4: The assessment factors of the modified EPA method for derivation of the NEC for predators (secondary poisoning).

Available information	Assessment factor
Less than 3 L(E)C ₅₀ s for different species and no NOECs	1,000
At least 3 L(E)C ₅₀ s for different species and no NOECs	100
3 NOECs for different species	10
Lowest NOEC value for chronic toxicity	10*

* This value is subsequently compared to the extrapolated value based on acute L(E)C₅₀s. The lowest one is selected.

BCFs for fish, mussels and earthworms

BCFs for fish, mussels and earthworms can be derived from experiments or using QSARs. According to Romijn et al. (1993) and Slooff (1992) preference is given to experimentally obtained BCFs for fish and mussels. If experimentally determined BCFs are not available for organic compounds, the BCF for fish and mussels is predicted from physico-chemical properties. The following QSARs which relate K_{ow} and the BCF for fish and mussels (on wet weight basis) are used (Mackay, 1982; Everts et al., 1992):

$$\text{fish: } BCF = 0.048 \cdot K_{ow} [//kg] \quad (10)$$

$$\text{musset: } BCF = 0.013 \cdot K_{ow} [//kg] \quad (11)$$

For metals, BCFs for fish and mussels are derived from values determined in laboratory tests.

BCFs for earthworms can also be obtained experimentally or estimated using QSARs. Romijn et al. (1994) showed that for dieldrin, DDT and pentachlorophenol geometric mean BCFs obtained from laboratory tests are less than 1. These BCFs were in good agreement with results reported by Connell and Markwell (1990). Romijn et al. (1994) concluded that the BCF for organic compounds is probably only dependent on soil characteristics and the lipid content of the organism and independent of the K_{ow} . Therefore, Slooff (1992) proposed to use a mean and maximum BCF of 1 and 10, respectively, for organic compounds. This approach is followed here. For metals, only experimentally determined BCFs for earthworms are used.

Correction factors

Dietary studies with birds and mammals are used to derive a NEC for predators. In these laboratory studies birds and mammals are usually fed with cereals. However, the caloric content of cereals is higher than the energy content of food consumed in the field, i.e. fish, mussels or earthworms. Hence, it is assumed that a predator has to consume a greater amount of fish, mussels or earthworms compared to cereals in order to obtain the same amount of energy. To correct for these differences in caloric content of the food, correction factors have to be applied (National Health Council, 1993; Van de Plassche, 1994). These correction factors are given in Table 5.

Table 5: Correction factors for extrapolation of dietary studies with birds and mammals to a NEC for predator

Species	Correction factor (CF)
Fish	0.32
Musset	0.20
Earthworm	0.23

The correction factors from Table 5 are used for mammals as well as birds because the caloric content of fodder for laboratory birds and mammals is almost the same: 14.8 and 16.8 kJ/g based on fresh weight for birds and mammals, respectively (Jongbloed et al., 1994).

2.3. 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 volatile nature it is assumed that exposure of human beings via air is a more important route than for ecosystems. The contribution of possible exposure through other routes is not taken into account in deriving the MPC for air. Therefore, only an MPC for the compartment air is derived for these compounds. Recently, a methodology was developed by which the exposure of human beings via several routes (e.g. food, air and drinking water) can be estimated (Mennes et al., 1995). By comparing the theoretical total daily intake (TDI) at environmental concentrations equal to the MPCs for the ecosystems and comparing this TDI with the acceptable daily intake (ADI) the protection level of human beings will be evaluated for the other compartments.

A minimum toxicity data set is defined that has to be met in order to derive an MPC for man (Rademaker et al., 1993^a). 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.

Non-carcinogenic compounds

The data used for derivation of an MPC for a non-carcinogenic compound have to meet several criteria. These are summarized in § 3 of Annex 1. The following procedure is applied for deriving an MPC (Rademaker et al., 1993^a):

1. All selected NOECs and LOECs are corrected for continuous exposure (see § 3 of Annex 1; formula 20). 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 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.

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, 1989).

If one or more elements of the minimum toxicity data set are lacking, a preliminary MPC for humans is derived (Rademaker et al., 1993^b). 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 20 (see § 3, Annex 1).

2.4 Procedure to derive MPCs for the compartments surface water, soil and air

The preceding paragraphs describe the procedures that are applied to derive MPC values on the basis of toxicological and ecotoxicological information. 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, different types of information have to be taken into account to set an MPC.

For *surface water* only the ecotoxicological effect data are taken into account in determining the MPC, for marine, fresh and groundwater. The ecotoxicological effect assessment includes direct and indirect effects. The MPC for direct effects is based on the preliminary or the refined effects assessment method, depending on the availability of data. The MPC for secondary poisoning (indirect effects) in the aquatic food chain is calculated using data on effects on birds and mammals using the mean bioconcentration factor for the most critical route (via fish or mussels). Subsequently, the MPC for surface water is derived by

comparing the MPC for direct effects and the MPC for secondary poisoning. In principle, the lowest of the two is selected. In addition, if relevant data from field tests or multi-species experiments are available, these are compared with the MPCs based on laboratory data. Data for water are expressed as dissolved concentrations, while usually total concentrations are or have been measured in environmental monitoring programmes. Dissolved concentrations can be calculated from total concentrations using the following equation:

$$C_{dissolved} = \frac{C_{total}}{1 + K_{p_{pm}} \cdot [pm]} \quad (12)$$

with:

$C_{dissolved}$	=	dissolved concentration in water (in mg/l)
C_{total}	=	total concentration in water (in mg/l)
$K_{p_{pm}}$	=	particulate matter/water partition coefficient (l/kg)
$[pm]$	=	concentration of particulate matter in water (kg/l) (in The Netherlands a particulate matter concentration of $30 \cdot 10^{-6}$ kg/l is used for surface water)

The procedure to derive an MPC for *soil* or *sediment* is similar to the one for water, i.e. the MPC is based only on ecotoxicological information. If secondary poisoning is critical, the MPC for secondary poisoning is used as the MPC for soil. In case no effect data on soil or benthic organisms are available, the MPC for direct effects is based on the MPC for surface water by applying the EP-method. Concentrations in soil or sediment are recalculated and normalized as described in Annex 1, § 2.1.

The MPC for *air* until now results from the human effect assessment as described in the previous section. 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 be used for instance to evaluate if emissions to air leading to certain air concentrations provide in the long term the necessary protection for soil ecosystems. The methodology is described in § 3.3.

Once the MPC values for the individual compartments have been derived it has to be assessed whether or not this set of risk limits needs to be harmonized. This harmonization procedure will be described in the next chapter.

Finally, it must be noted that the procedures described in this chapter must be regarded in that they provide a way to derive MPC values for a large number of substances in a consistent and systematically manner. This does not mean that there is no allowance to deviate from these procedures. For all chemicals a case-by-case assessment is made in setting the final MPC values, taking into account the number and reliability of the underlying data. Part II of this report will demonstrate that in many cases the standard procedures were departed from to a small or sometimes larger extent.

3. HARMONIZATION OF MPCs

3.1 The harmonization principle

The effect-oriented environmental policy in most countries is still characterized by a compartmental approach. Risk limits or quality standards are determined for the compartments air, water and soil individually, notwithstanding the transport of chemicals from one compartment to another as well as the effects that can be caused in other compartments than those to which the chemicals have been released. Thus, harmonization of these standards is highly necessary because of the fact that (1) releases of chemicals to water and soil can, after volatilization, lead to deleterious effects in the air, either to man or to parts of the ecosystems and (2) because the air is a very important transportation medium for many, also relatively non-volatile, chemicals which may affect the quality of water and soil. Hence, achieving concentrations lower than the quality criterion for one compartment does not necessarily mean that a 'safe' concentration in another compartment can be obtained and maintained.

In order to test if independently-derived MPCs are coherent a special harmonization procedure has been developed. In this procedure it is assumed that the emissions, both within the area of concern and outside, have been controlled to such a level that the concentration in the so-called primary compartment has become equal to the MPC. This implies that the emissions have remained constant for a sufficiently long period of time that all concentrations in the environment, in the primary compartment as well as in the secondary compartments, have become constant in time (steady-state). The coherence criterion is tested by comparing the concentrations at steady-state in the secondary compartments with the MPCs that have been proposed for the secondary compartments. If the analysis indicates that maintaining the primary compartment at MPC level is likely to result in MPC exceedance in any of the secondary compartments, the set of MPCs must be considered incoherent, since it is not likely that co-existence of concentrations at these MPC levels can be achieved.

In order to harmonize the quality standards for *water and soil* and for *water and sediment* the equilibrium partitioning concept is applied. This approach assumes that in the long term concentrations in water and sediments or in groundwater and soil are expected to approach equilibrium. Hence, sediment/water and soil/water partition coefficients are applied to convert quality standards that have been derived for water into standards for sediment and soil, respectively (Van de Meent et al., 1990). The equilibrium partitioning concept may not be applied for the harmonization of *water and soil* quality standards with standards 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 harmonization between air on the one hand and soil and water on the other hand (Van de Meent and de Bruijn, 1995).

3.2 Harmonization of MPCs for air, water and soil

3.2.1 Introduction

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.

3.2.2 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 harmonization of MPCs, SimpleBox represents the behaviour of micropollutants in a model environment, resembling The Netherlands.

A schematical representation of the model is shown in Figure 5 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 Appendix 5. 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 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, the octanol/water partition coefficient and degradation rates in air, water, and soil. The selection of these data is described in § 4 of Annex 1. Currently, a series of studies are running to validate the SimpleBox model with several model compounds, as a result of the advice that the National Health Council has given (National Health Council, 1995).

Figure 5: 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.

3.2.3 Procedure

When the individual MPCs for the different compartments have been derived and the physico-chemical data are collected, the harmonization of the MPCs can be carried out. The objective of the harmonization 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 harmonization 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 compart-

ments 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:

$$\frac{C_{air}}{C_{water}} = \frac{H_c}{R \cdot T} \cdot 1,000 \quad (13)$$

$$\frac{C_{soil}}{C_{water}} = K_{p_{soil}} \quad (14)$$

$$\frac{C_{air}}{C_{soil}} = \frac{H_c}{R \cdot T \cdot K_{p_{soil}}} \cdot 1,000 \quad (15)$$

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)
$K_{p_{soil}}$	=	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 second-

ary 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 5, 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 harmonization of MPC values for air, water and soil has recently been published (Van de Meent and de Bruijn, 1995) and has been applied to some 30 volatile organic chemicals (Van de Plassche and Bockting, 1993).

3.3 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 standards 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:

$$CritCONC_{air} = \frac{MPC_{soil}}{SSCR_{soil/air}} \quad (16)$$

and

$$CritCONC_{rain} = CritCONC_{air} \cdot ScavRatio \quad (17)$$

with:

$CritCONC_{air}$	=	critical concentration in air in g/m^3
MPC_{soil}	=	maximum permissible concentration in soil in g/kg (dry weight)
$SSCR_{soil/air}$	=	steady-state concentration ratio soil/air in m^3/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 m_{air}^3/m_{rain}^3

The SimpleBox model is originally developed for organic substances. Application of the model for metals in order to calculate SSCRs is possible but needs some specific parameters settings for $\log K_{ow}$, vapour pressure, scavenging ratio, fraction aerosol bound metal and degradation rates.

The model describes a reference environment, in this case The Netherlands. Therefore, the $CritCONC_{air}$ and the $CritCONC_{rain}$ will relate to relatively large geographic areas but not necessarily to smaller geographic areas.

3.4 Harmonization of MPCs with the EP-method

Usually, the EP-method is applied to derive MPCs in sediment or soil from the

MPC in surface water when no ecotoxicity data on benthic or soil organisms are available (see section 2.2.4). In that case the EP-method is used as an indirect method to derive MPCs for sediment and soil and harmonization of these values has been done already. In case sufficient data are available to derive MPC values for surface water as well as for sediment and/or soil individually, these values can in turn be harmonized by means of the EP-method. The formulas used for this application of the EP-method are identical to the ones mentioned in § 2.2.4 (formulas 6 and 7) and will therefore not be repeated here.

If MPCs are available based on ecotoxicological data (direct and indirect effects) as well as by the use of the equilibrium partitioning method, both MPCs are compared. Noteworthy is that the K_p (especially for metals) must be critically reviewed, before a meaningful comparison between MPCs based on ecotoxicity data and equilibrium partitioning is possible. For soil, in general, the MPC values based on ecotoxicological effect data (indirect or direct) are preferred. However, if the MPC for surface water is based on a relatively large data set containing chronic data on several taxonomic groups while the MPC for soil is based on a limited data set, the MPC based on equilibrium partitioning may, on a case by case basis, be given more weight and be chosen as the MPC for soil.

3.5 Comparison of MPC values with background concentrations

Metals (as well as various nutrients and some organic compounds) naturally occur in surface water, sediment, soil and groundwater. The derivation of MPCs for naturally-occurring compounds is described in § 2.2.2.3. The concentration of naturally-occurring compounds can differ from location to location (naturally-occurring variation) and can reach high levels. Some compounds are even essential for aquatic or soil organisms to survive and therefore may influence the biodiversity (De Bruijn and Denneman, 1992).

To determine natural background concentrations of metals in surface water, relatively clean surface water and analysis methods with a low detection limit are necessary. Because clean surface water is lacking in The Netherlands, measured concentrations of metals in samples from brooks in relatively clean areas in the Northern European Lowland are used. Hereby, the assumption is made that the Northern European Lowland is representative for The Netherlands (De Bruijn and Denneman, 1992; Zuurdeeg et al., 1992).

For background concentrations of metals in soil, measured concentrations in soil samples from a large number of relatively unpolluted natural areas in The Netherlands are used. If sufficient data are available, the relation between the background concentrations of the metals and the organic matter and/or clay content is determined by multiple regression analysis, resulting in so called 'reference lines' (see also section 2.1 in Annex 1). This allows a naturally-occurring variation in the concentrations of these metals in soil. Because the measured concentrations within one location can vary, it is very important that reference lines are based on measured concentrations derived with the same analytical methods.

Background concentrations in groundwater are based on measured concentrations from the 'Dutch groundwater quality monitoring network' (Duijvenbooden and Prins, 1991). If a sufficient number of data ($n > 50$) is available, the 90th-percentile value is calculated and regarded as the background concentration (De

Bruijn and Denneman, 1992; Van den Hoop et al., 1995).

ANNEX 1: EVALUATION OF (ECO)TOXICOLOGICAL AND PHYSICO-CHEMICAL DATA

1. Introduction

Physico-chemical and (eco)toxicological data are needed to derive MPCs for the different compartments and to carry out the harmonization procedure as described in the previous chapters. These data are obtained by literature search. Which data are needed and for what purpose, will be presented in the following paragraphs.

The quality of data has to be assessed after the relevant literature is collected. This process involves:

- A review of individual data elements with respect to how the study was conducted and how the results were interpreted. This concerns the reliability of the test, i.e. both methodology and description.
- A critical selection (and rejection) of data in its proper context and in accordance with the purpose of the review, i.e. assessment of the usefulness.

For assessing the reliability, internationally accepted test guidelines such as those of the Organisation for Economic Co-operation and Development (OECD) are used as a point of reference: selected studies have to be performed according to these guidelines (OECD, 1981^a). The reality is, however, that many studies have not been conducted based on such guidelines. Moreover, for many tests no guidelines are available. If the latter is the case, the reliability is assessed using expert criteria (CSR, 1996).

2. Evaluation of ecotoxicological data

Ecotoxicological data for saltwater as well as freshwater organisms, benthic and soil organisms, birds and mammals are used to derive an MPC based on direct effects for water, sediment, soil and air (see section 2.2). For deriving an MPC based on indirect effects (see section 2.2.5) also BCFs for fish, mussels or earthworms are needed.

Usually, most data are from single-species studies carried out in the laboratory. Sometimes field studies are available. A set of criteria of Emans et al. (1992) is used to assess the reliability of the field studies.

Only those ecotoxicological data are selected which meet parameters that affect the species on the level of population. Whether other effect parameters studied are relevant is decided on a case by case basis. Examples of relevant parameters are mortality, growth, photosynthesis and reproduction (including effects on reproductive organs, spermatogenesis, fertility, pregnancy rate, number of eggs produced, egg fertility, hatchability) (Slooff, 1992).

As MPCs are derived using short-term L(E)C₅₀s and long-term NOECs these endpoints are extracted from ecotoxicological literature. The following procedures are used for deriving a long-term NOEC:

- If the NOEC is based on a statistical method these results are used: the highest concentration tested, not differing from the control at $P < 0.05$, is regarded as the NOEC.

- If no statistical method is applied the concentration showing less than 10% effect is considered as the NOEC. However, there must be a distinct concentration-effect relationship.
- If effects are observed at the lowest test concentration the LOEC is converted into a NOEC as follows:
 - a) LOEC > 10 to 20% effect: the NOEC = LOEC/2;
 - b) LOEC ≥ 20% effect and a distinct concentration-effect relationship: the EC10 is calculated or extrapolated and regarded as the NOEC;
 - c) LOEC ≥ 20% with no distinct concentration-effect relationship:
 - LOEC 20 to 50% effect: NOEC = LOEC/3;
 - LOEC ≥ 50% effect: NOEC = LOEC/10.

If other results are available within the same taxonomic group with obvious concentration-effect relationships, these are used to verify the above mentioned factors. If for instance an acute/chronic ratio is available within the same taxonomic group this ratio is used instead of one of the factors mentioned above.

- The 'Toxische Grenzkonzentration' (TGK) or Toxic Threshold of 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 value is used as the NOEC. If a MATC is presented as one value the NOEC is calculated as MATC/2 (Van de Plassche et al., 1992).
- Studies with mammals and birds exposed for less than 1 month are regarded as short term. A long-term NOEC is derived by dividing the short term NOEC by 10 (Romijn et al., 1993).
- From chronic tests on mammals with a test duration of two years or more, no NOEC for mortality is derived because usually more than 20% mortality occurs in the second year which is probably not caused by the test compound (Romijn et al., 1993).

In ecotoxicological studies with essential elements it can theoretically occur that the effects observed are caused by element limitation instead of toxic effects. To prevent this, special attention is paid to studies resulting in low NOEC or L(E)C50 values for the metals antimony, cobalt, molybdenum, selenium, vanadium, chromium, copper and zinc. Studies resulting in low NOEC or L(E)C50 values have been specifically evaluated paying attention to the following criteria:

- Only studies in which there is a concentration-effect relationship are used. This criterion is applied to be sure that NOECs are based on effects due to toxic effects instead of limitation.
- The NOEC should be derived after a sufficiently long exposure period and in the toxic concentration band. This criterion is considered especially for studies in which the test-organisms are cultured in media containing low levels of trace metals.

In the following paragraphs some special aspects with respect to the evaluation of ecotoxicological data will be described.

2.1 Normalization of data for soil and benthic organisms

Soils used in ecotoxicological tests differ in characteristics like organic matter and clay content, soil pH, soil moisture content. The bioavailability of the test

compound, and therefore the observed toxicity is influenced by these soil properties. This means that results from different test soils cannot be compared as such. Hence, data have to be normalized using relationships which describe the bioavailability of chemicals in soils or approximations of it. Therefore results are converted to a standard soil, which is defined as a soil with a clay and organic matter content of 25% and 10%, respectively.

For non-ionic organic compounds it is assumed that bioavailability is determined by the organic matter content, only. This has been shown e.g. for earthworms for short term tests with chlorobenzenes and chloroanilines (Van Gestel and Ma, 1990; Van Gestel et al., 1991). NOECs and $L(E)C_{50}$ s are corrected according to the formula:

$$NOEC \text{ or } L(E)C_{50(standard)} = NOEC \text{ or } L(E)C_{50(exp)} \cdot \frac{f_{om(standard)}}{f_{om(exp)}} \quad (18)$$

with:

$f_{om(standard)}$ = fraction organic matter in standard soil, i.e. 10%;
 $f_{om(exp)}$ = fraction organic matter in experimental soil.

For metals it is assumed that bioavailability is influenced by the organic matter and clay content. Equations derived for the relationship between background levels of chemicals in Dutch reference soils and clay and/or organic matter content are used (VTCB, 1986; Van Straalen and Denneman, 1989; De Bruijn and Denneman, 1992). These equations are called 'soil type correction factors' and are presented in the table below.

Name	Soil type correction factors (R)
chromium	50 + 2L
nickel	10 + L
copper	15 + 0.6 (L + H)
zinc	50 + 1.5 (2L + H)
cadmium	0.4 + 0.007 (L + 3H)
mercury	0.2 + 0.0017 (2L + H)
lead	50 + L + H
arsenic	15 + 0.4 (L + H)
barium	30 + 5L
beryllium	0.4 + 0.024L
cobalt	2 + 0.28L
tin	4 + 0.6L
vanadium	12 + 1.2L
L = lutum (clay) H = humus (organic matter)	

Subsequently, the following formula is used to normalize toxicity data to a standard soil of 25% clay and 10% organic matter:

$$NOEC \text{ or } L(E)C_{50(standard)} = NOEC \text{ or } L(E)C_{50(exp)} \cdot \frac{R_{(standard)}}{R_{(exp)}} \quad (19)$$

with:

- $R_{(standard)}$ = reference value for standard soil: value calculated using a clay content of 25% and an organic matter content of 10%,
- $R_{(exp)}$ = value determined for the experimental soil, calculated using the clay (L) and organic matter (H) content of the soil used in the experiment.

An example for lead is given in footnote 1. It is realized that the 'soil type correction factors' are not ideal as an important factor such as pH is not included. Van Gestel et al. (1995) conclude in a review on the influence of soil properties on the toxicity of metals on soil invertebrates that pH is the most important factor followed by the organic matter content and cation exchange capacity. But for each metal another combination of factors seems to determine bioavailability. More research is needed to quantify these factors. At the moment normalization by means of the 'soil type correction factors' is considered the best available option.

2.2 Normalization of data for organisms exposed via air

For the compartment air often only toxicity data on mammals are available (Rademaker and van Gestel, 1993). Sometimes toxicity data for other organisms like birds, insects or plants are present. The reliability of these data has to be judged on a case by case basis because no test methods and/or international accepted test guidelines for air exist at the moment. Recently, test methods have been proposed for plants and arthropods (Tonneijk and Van Dijk, 1993; Rademaker and Van Gestel, 1993).

In toxicity studies with organisms exposed via air the exposure regime is in most tests discontinuous, e.g. 6 hours per day and 5 days per week. As the MPC in air is based on continuous exposure all $L(E)C_{50}$ s and NOECs are corrected applying the following formula (RIVM, VROM and WVC, 1994):

$$NOEC \text{ or } L(E)C_{50} = NOEC \text{ or } L(E)C_{50(exp)} \cdot \left(\frac{d}{7}\right) \cdot \left(\frac{h}{24}\right) \quad (20)$$

with:

- d = number of days exposed per week
- h = number of hours exposed per day

2.3 Effect data needed for the assessment of secondary poisoning

In order to take into account indirect effects on top predators exposed via the food chain, ideally long-term toxicity data have to be available for these organisms like hawks, owls and weasels. However, laboratory experiments with top predators are rare: for birds most laboratory toxicity tests have been carried out on hens, pheasants and quails. Usually these tests are dietary studies in which the test organism is fed with cereals. As described in section 2.2.5, NOECs derived from these studies are corrected and used for the whole group of top predators.

¹ Lead; artificial soil: 10% clay (L) and 8% organic matter (H), the measured concentration is 10 mg/kg. The concentration in standard soil is $10 \text{ mg/kg} \cdot \{(50 + 25 + 10)/(50 + 10 + 8)\} = 37.5 \text{ mg/kg}$.

Results of dietary studies with birds or mammals are often expressed in mg/kg body weight. These NOECs have to be converted to mg/kg food to derive an MPC (see section 2.2.5). BW/DFI factors (BW = body weight; DFI = daily food intake) are used for this conversion. An overview of BW/DFI factors used is given in the table below for several test organisms.

Organisms	Body weight / Daily food intake (BW/DFI) 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
Rattus norvegicus (rat)	20
Mustela vison (mink)	10

2.4 Bioconcentration factors

BCFs for fish, mussels and earthworms are needed to derive an MPC based on indirect effects. The following criteria are used for selecting BCFs measured in laboratory studies with freshwater and saltwater fish and bivalves:

- 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. The minimal exposure time is the time needed to reach 80% of the steady-state: the T80. This T80 value is calculated based on the log K_{ow} (OECD, 1981^b), but it must be noted that the T80 also depends on body weight and lipid content of the organism.
- No signs of overt toxicity should have been observed: if mortality occurs, the test concentration is excluded, while if nothing is reported on mortality, all test concentrations higher than 20% of the 96 hours L(E)C₅₀s are excluded.
- Only studies reporting BCFs for whole body based on wet weight are selected. For mussels, BCFs for whole body are based on the soft parts, i.e. without the shell.
- If more than one value is determined on a single species, a geometric mean is calculated on this species. Further, an overall geometric mean BCF is calculated from the values of different species.

3. Evaluation of toxicity data

For the derivation of an MPC for human beings a full toxicological profile for each substance has to be present. These data are mainly derived from laboratory studies with mammals. After collection of reliable data from toxicity tests, those data are selected for further consideration in which relevant toxicological endpoints like carcinogenic effects, mutagenic effects, reproductive effects, teratogenic effects and systemic effects are tested. These may concern mortality, growth, organ weight, haematological changes and (histo)pathological and biochemical changes (Slooff, 1992). Data from human case-controlled studies can also be used for the derivation of an MPC for humans. However,

these studies are very scarce and need a case by case assessment to judge whether the results can be used.

As stated in paragraph 2 until now only MPCs in air have been derived for human beings. This means that toxicity studies via the inhalatory route are used. Selected toxicity data are corrected for a full time exposure applying the formula 19.

The following additional criteria are used:

- Exposure time has to be sufficiently long: only those (sub)chronic inhalation toxicity studies are selected with an exposure time of 4 hours per day and 5 days per week, or more. Inhalation studies for which no information is available on the exposure time, are excluded.
- Concentrations at which maternal toxicity occurs are not regarded as teratogenic effects. Teratogenic effects are defined as irreversible structural effects on the foetus only.
- Toxicity tests in which animals are orally exposed can also be used. Based on NOECs or LOECs from oral studies, an oral MPC for humans is derived. Subsequently this oral concentration can be converted into an inhalation concentration using the following formula (RIVM, WVC and VROM, 1994):

$$\text{inhalation NOEC} \cdot IR \cdot t \cdot B_{inh} = \text{oral NOEC} \cdot BW \cdot B_{oral} \quad (21)$$

with:

- IR = inhalation rate (0.83 m³/h)
- t = duration of exposure per day (24 h)
- B_{inh} = inhalation bioavailability (set at 75 %)
- BW = body weight humans (70 kg)
- B_{oral} = oral bioavailability (set at 100 %)

4. Evaluation of physico-chemical data

In order to apply extrapolation (see chapter 3) and harmonization methods (see chapter 4), several physico-chemical characteristics of the substance are needed. The most important ones are:

- the octanol/water partition coefficient (K_{ow})
- the soil/water partition coefficient (K_p)
- the sediment/water partition coefficient (K_p)
- the Henry's law constant (H_c)
- degradation in air
- degradation in water and soil
- the vapour pressure
- solubility in water.

4.1 Octanol/water partition coefficient

Octanol/water partition coefficients obtained by the slow-stirring method are preferred (De Bruijn et al., 1989). If not available, K_{ow}s are selected from the MEDCHEM database using the so called 'star values': the value that is considered most reliable in the data-base is indicated with a star.

Besides a large number of K_{ow} values from the literature the MEDCHEM database contains a routine for estimation of K_{ow} s based on structural properties of the compound (ClogP method). K_{ow} s calculated with the ClogP method are less reliable than experimental values, but in an evaluation of the system Verhaar and Hermens (1990) concluded that this estimation method normally leads to reasonable values.

4.2 Soil/water and sediment/water partition coefficient

The soil/water and the sediment/water partition coefficient are defined as the ratio of the concentration of a chemical in the solid phase (sorbed fraction) and sediment phase, divided by its concentration in the water phase, respectively.

Organic compounds

The determination of partition coefficients for organic compounds can be based on experiments and estimation methods. K_p values are preferably based on values from batch experiments (Bockting et al., 1993). In these experiments the absorbed fraction is calculated from the decrease of the aqueous concentration in a water-soil/sediment system.

K_p s are calculated from the K_{oc} according to:

$$K_p = K_{oc} \cdot f_{oc} \quad (22)$$

with:

f_{oc} = fraction organic carbon in soil or sediment; f_{oc} is fixed at 5% (Slooff, 1992).

If no experimental data are available the K_p is estimated using the following formulas:

$$\log K_{oc} = a \log K_{ow} + b \quad (23)$$

with:

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

Gerstl (1990) derived regression equations as given in formula 22 for compounds from 16 chemical groups, based on a large database. These equations relating K_{ow} and K_{oc} are presented in the table below.

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

If a chemical does not belong to one of the classes mentioned in this table, the relation of DiToro et al. (1991) is used:

$$\log K_{oc} = \log K_{ow} [l/kg] \quad (24)$$

Some organic compounds contain acidic groups (e.g. hydroxyl or carboxyl groups) from which a proton can dissociate. The negatively charged ions formed are less hydrophobic than their uncharged parent acids. Therefore, a pH-dependent partition coefficient is sometimes calculated from the K_{ow} and pK_a (Van de Meent et al., 1990). Comparison of experimental and calculated K_{oc} s by Bockting et al. (1993) showed that the formulation of pH-dependent K_{oc} s leads to a severe underestimation of adsorption. Therefore, DiToro's equation is used for such compounds if no experimental values are available.

Metals

The partition coefficient for metals can only be derived experimentally, since no general estimation model is available (Bockting et al., 1992). For sediment, batch experiments are often lacking. For this reason K_p s for sediment are derived from measurements of the metal content of particulate matter in rivers and corresponding water samples. The organic matter and clay content, however, are higher in particulate matter than in sediment. Therefore the K_p s for particulate matter are divided by a factor 1.5 to obtain K_p values for sediment (Van de Meent et al., 1990).

4.3 The Henry's law constant

The Henry's law constant or Henry coefficient (H_c) describes the equilibrium distribution of a chemical over the gas and water phase. It can experimentally be determined or estimated from the water solubility and vapour pressure:

$$H_c = \frac{(\text{vapour pressure})}{(\text{solubility})} \text{ (Pa}\cdot\text{m}^3/\text{mol)} \quad (25)$$

Preferably H_c values measured at 10°C are used, since this is the temperature of the water used in the model SimpleBox. Ten Hulscher et al. (1992) and Ashworth (1988) observed a doubling of experimental H_c values for e.g. chlorobenzenes, PCBs and PAHs for every 10 °C temperature increase. Therefore H_c s determined at 20 or 25 °C (or calculated from vapour pressures and water solubility) are lowered with a factor 2 or 3, respectively.

4.4 Degradation in air

Organic compounds can be removed from the troposphere by photolysis and reaction with OH and NO₃ radicals, and with O₃. According to Atkinson (1985) it is widely recognized that the OH radical is the dominant reactive species in the degradation of organic compounds in both the natural and polluted troposphere. Degradation rate constants are taken from an extensive review of Atkinson (1985). An OH radical concentration of 10⁶ molecules/cm³ is used to calculate the fraction of the compound degraded per day. This value is recommended by De Leeuw (1993) as typical for the northern hemisphere.

4.5 Degradation in water and soil

The potential for biodegradation is often determined in biodegradation tests where the compound is either assigned as readily biodegradable or not readily biodegradable. The harmonization model attributes a degradation rate proportional to the concentration of bacteria in water (degradation in soil and sediment is assumed to occur only for the interstitial water dissolved fraction of the chemical). Pseudo first order degradation rate constants are obtained by extrapolation from the results of standard screening tests for ready biodegradability in water (Struijs and van den Berg, 1992).

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APPENDIX 1: ABBREVIATIONS

ALARA	as low as reasonably achievable
AVS	acid volatile sulphide
BCF	bioconcentration factor
BW	body weight
CF	correction factor
CritCONC	critical concentration
DFI	daily food intake
d	number of days exposed per week
DCV	duration corrected value
EC ₅₀	effect concentration at which 50% of the tested species show effect
EDF	empirical distribution function
EPA	Environmental Protection Agency
EP-method	equilibrium partitioning method
EQS	environmental quality standard
f _{oc}	fraction organic carbon
f _{om}	fraction organic matter
Fu(x)	fraction of species unprotected at concentration x (currently the abbreviation PAF is used)
h	number of hours exposed per day
H	humus (organic matter)
H _c	Henry's law constant
HC5	Hazardous Concentration that potentially affects 5% of the species
I	tumour incidence for humans
IR	inhalation rate
K _{oc}	organic carbon/water partition coefficient
K _{ow}	octanol/water partition coefficient
K _p	sediment/water, soil/water or particulate matter/water partition coefficient
MATC	maximum acceptable toxicant concentration
MPC	maximum permissible concentration
NC	negligible concentration
NEC	no-effect concentration
NEL	no-effect level
NEPP	National Environmental Policy Plan
NOEC	no observed effect concentration
L	lutum (clay)
LC ₅₀	lethal concentration at which 50% of the tested animals die
LOEC	lowest observed effect concentration
OECD	Organisation for Economic Co-operation and Development
pKa	negative logarithmic value of the equilibrium constant for an acid dissociation reaction
QSAR	quantitative structure-activity relationship
R	reference value
SSCR	steady-state concentration ratio
TGK	Toxische Grenzkonzentration
TDI	total daily intake
UF	uncertainty factor

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APPENDIX 2: GLOSSARY

Adverse effect	: negative change in morphology, physiology, growth, development or lifespan of an organism
Available fraction	: in soil: the fraction of the metal that is extractable from the substrate with chemical (e.g.: neutral salt, water extraction) or physical means (shaking, interstitial water collection), and that is generally considered to be a better estimate for the fraction that is available for organisms than the total concentration. In water: the dissolved fraction of the total concentration.
Background concentration	: the concentration that is present in rural sites due to natural causes only. (In The Netherlands it is impossible to find locations at which background concentrations can be measured)
Bioaccumulation	: the net result of the uptake, distribution and elimination of a substance due to all routes of exposure
Bioconcentration	: the net result of the uptake, distribution and elimination of a substance due to water-borne exposure
Biomagnification	: the accumulation and transfer of chemicals via the food web (e.g. algae-invertebrate-fish-mammal) due to ingestion, resulting in an increase of the internal concentration in organisms at the succeeding trophic levels.
Biota	: all living organisms
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
Effect	: the change in the state or dynamics of an organism or other ecological system resulting from exposure to a chemical or other stressor
Equilibrium	: condition in which no further change occurs in time and in which phases have concentrations such that they experience no tendency for net transfer of mass
Food chain	: sequence of transfer of matter and energy in the form of food from organism to organism in ascending or descending trophic levels

Genotoxicity	: ability to cause damage to genetic material or an adverse effect in the genome; such damage can be mutagenic and/or carcinogenic
Hazard (toxic)	: the potential of a substance to cause adverse effects at a particular level of exposure
Leaching	: transfer of a chemical from the top layer of soil to the ground water
LC50	: median Lethal Concentration: a statistically-derived concentration that can be expected to cause death in 50% of animals exposed for a specified time
Mutagenicity	: ability of a physical, chemical or biological agent to induce heritable changes (mutations) in the genotype in a cell as a consequence of alterations or loss of genes or chromosomes (or parts thereof)
NEC	: no-effect concentration derived from extrapolations of results from dietary laboratory toxicity test with animals representative for predators (in mg/kg food)
NOEC	: No-Observed Effect Concentration: the highest concentration that does not cause any observed and statistically significant adverse effects on the organism compared to the controls
NOEL	: No-Observed Effect Level: see NOEC
Partition coefficient	: ratio of the distribution of a substance between two phases when the heterogeneous system (of two phases) is at equilibrium; the ratio of concentrations (or, strictly speaking, activities) of the same molecular species in the two phases is constant at constant temperature
Predator	: animal that feeds on other animals, i.e. a secondary consumer (parasites are excluded)
Primary compartment	: compartment in which emission of a chemical takes place
Reference lines	: in case of soil, for all metals so-called reference lines were derived by correlating measured ambient background concentrations (total concentrations in the soil-matrix) at a series of remote rural sites in The Netherlands to the percentage lutum (%L) and the organic matter content (%H) of these soils.
Risk	: the probability of a substance to cause adverse effects on man or the environment

Risk assessment	: determination of the relation between the predicted exposure and adverse effects in four major steps: hazard identification, dose-response assessment, exposure assessment and risk characterization
Risk management :	decision-making process involving considerations of political, social, economic, and engineering factors with relevant risk assessments relating to a potential hazard so as to develop, analyse, and compare regulatory options and to select the optimal regulatory response for safety from that hazard
Safety	: reciprocal of risk: practical certainty that injury will not result from a hazard under defined conditions
Secondary compartment	: the compartment to which a compound will diffuse to or transported to, to reach a steady-state situation
Secondary poisoning	: the product of biomagnification and toxicity
Standard soil	: in The Netherlands a hypothetical soil, defined to contain 25% lutum or clay and 10% organic matter, is indicated a standard soil. The standard soil is used to normalize toxicity and exposure data
Steady-state	: a condition in which all concentrations in different compartments are constant in time but in which the concentrations are not necessarily in thermodynamic equilibrium
Suspended matter	: all abiotic colloidal or macromolecular material that is not truly dissolved
Threshold value	: the lowest exposure level in one test at which the most critical effect is occurring
Uptake	: the amount of a substance which has been absorbed, i.e. which has passed into the systemic circulation of an organism

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APPENDIX 3: FORMULAS

Formula number	Formula	Page number
1	$Fu(x) = \frac{1}{(1 + \exp(\frac{\alpha - x}{\beta}))}$	14
2	$x = \alpha - \beta \ln \{(1 - Fu)/Fu\}$	14
3	$MPC = MPA + Cb$	16
4	$NA = \frac{MPA}{100}$	16
5	$NC = NA + Cb$	16
6	$MPC_{sediment} = K_p \cdot MPC_{surface\ water}$	19
7	$MPC_{soil} = K_p \cdot MPC_{surface\ water}$	20
8	$MPC_{sec.pois.} = NEC_{predators} \cdot \frac{CF}{BCF_{fish/mussel}} \text{ water:}$	21
9	$MPC_{sec.pois.} = NEC_{predators} \cdot \frac{CF}{BCF_{earthworm}} \text{ soil:}$	21
10	$fish: BCF = 0.048 \cdot K_{ow} [l/kg]$	22

Formula number	Formula	Page number
11	$\text{musset. BCF} = 0.013 \cdot K_{ow} [l/kg]$	22
12	$C_{dissolved} = \frac{C_{total}}{1 + Kp_{pm} \cdot [pm]}$	25
13	$\frac{C_{air}}{C_{water}} = \frac{H_c}{R \cdot T} \cdot 1,000$	29
14	$\frac{C_{soil}}{C_{water}} = Kp_{soil}$	29
15	$\frac{C_{air}}{C_{soil}} = \frac{H_c}{R \cdot T \cdot Kp_{soil}} \cdot 1,000$	29
16	$CritCONC_{air} = \frac{MPC_{soil}}{SSCR_{soil/air}}$	31
17	$CritCONC_{rain} = CritCONC_{air} \cdot ScavRatio$	31
18	$NOEC \text{ or } L(E)C_{50(standard)} = NOEC \text{ or } L(E)C_{50(exp)} \cdot \frac{f_{om(standard)}}{f_{om(exp)}}$	iii
19	$NOEC \text{ or } L(E)C_{50(standard)} = NOEC \text{ or } L(E)C_{50(exp)} \cdot \frac{R_{(standard)}}{R_{(exp)}}$	iii

Formula number	Formula	Page number
20	$NOEC \text{ or } L(E)C_{50} = NOEC \text{ or } L(E)C_{50(\text{exp})} \cdot \left(\frac{d}{7}\right) \cdot \left(\frac{h}{24}\right)$	iv
21	$\text{inhalation NOEC} \cdot IR \cdot t \cdot B_{inh} = \text{oral NOEC} \cdot BW \cdot B_{oral}$	vi
22	$Kp = K_{oc} \cdot f_{oc}$	vii
23	$\log K_{oc} = a \log K_{ow} + b$	vii
24	$\log K_{oc} = \log K_{ow} [l/kg]$	viii
25	$H_o = \frac{(\text{vapour pressure})}{(\text{solubility})} (Pa \cdot m^3/mol)$	ix

The abbreviations used in the above mentioned formulas are given in Appendix 1.

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APPENDIX 4: THE QSAR EQUATIONS FOR CHEMICALS ACTING BY NARCOSIS

QSAR equations can be applied for chemicals acting by narcosis. The mechanism of narcosis is nonspecific; 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. Van Leeuwen et al. (1992) have selected 19 QSARs for chronic toxicity for aquatic species. These are given in the following table, while the $\log K_{ow}$ dependent HC5, and thus the MPC, can be read from the subsequent table:

Species	QSAR (NOEC expressed as mol/l)
Bacteria	
<i>Clostridium botulinum</i>	$\log \text{NOEC} = -0.82 \log K_{ow} - 0.29$
<i>Bacillus subtilis</i>	$\log \text{NOEC} = -0.64 \log K_{ow} - 1.03$
<i>Pseudomonas putida</i>	$\log \text{NOEC} = -0.64 \log K_{ow} - 1.60$
<i>Photobacterium phosphorum</i>	$\log \text{NOEC} = -0.68 \log K_{ow} - 1.52$
Algae	
<i>Skeletonema costatum</i>	$\log \text{NOEC} = -0.72 \log K_{ow} - 1.42$
<i>Scenedesmus subspicatus</i>	$\log \text{NOEC} = -0.86 \log K_{ow} - 1.41$
<i>Selenastrum capricornutum</i>	$\log \text{NOEC} = -1.00 \log K_{ow} - 1.71$
Fungi	
<i>Saccharomyces cerevisiae</i>	$\log \text{NOEC} = -0.78 \log K_{ow} - 0.35$
Protozoans	
<i>Tetrahymena pyriformis</i>	$\log \text{NOEC} = -0.80 \log K_{ow} - 1.28$
Coelenterates	
<i>Hydra oligactis</i>	$\log \text{NOEC} = -0.86 \log K_{ow} - 2.05$
Molluscs	
<i>Lymnaea stagnalis</i>	$\log \text{NOEC} = -0.86 \log K_{ow} - 2.08$
Arthropods	
<i>Nitocra spinipes</i>	$\log \text{NOEC} = -0.78 \log K_{ow} - 2.14$
<i>Daphnia magna</i>	$\log \text{NOEC} = -1.04 \log K_{ow} - 1.70$
<i>Aedes aegypti</i>	$\log \text{NOEC} = -1.09 \log K_{ow} - 1.36$
<i>Culex pipiens</i>	$\log \text{NOEC} = -0.86 \log K_{ow} - 1.98$
Fish	
<i>Pimephales promelas</i> / <i>Brachydanio rerio</i>	$\log \text{NOEC} = -0.87 \log K_{ow} - 2.35$
Amphibia	
<i>Ambystoma mexicanum</i>	$\log \text{NOEC} = -0.88 \log K_{ow} - 1.89$
<i>Rana temporaria</i>	$\log \text{NOEC} = -1.09 \log K_{ow} - 1.47$
<i>Xenopus laevis</i>	$\log \text{NOEC} = -0.90 \log K_{ow} - 1.79$

Based on these QSARs, NOEC values can be calculated for every $\log K_{ow}$ value. Subsequently the HC5 is calculated under the assumption of a log-logistic distribution according to the method of Aldenberg & Slob (1993) for narcotic chemicals as a function of K_{ow} . HC5-values are presented in the following table for $\log K_{ow}$ -values ranging from -1 to 7 at intervals of 0.1.

log K _{ow}	log HC5			log K _{ow}	log HC5		
	dissolved (mol/l)	sediment (mol/kg)	total (mol/l)		dissolved (mol/l)	sediment (mol/kg)	total (mol/l)
-1.00*	-1.69	-4.21	-1.69	3.00	-5.31	-3.84	-5.31
-0.90*	-1.77	-4.19	-1.77	3.10	-5.41	-3.84	-5.41
-0.80*	-1.85	-4.17	-1.85	3.20	-5.51	-3.84	-5.51
-0.70*	-1.93	-4.15	-1.93	3.30	-5.61	-3.83	-5.61
-0.60*	-2.01	-4.14	-2.01	3.40	-5.71	-3.83	-5.71
-0.50*	-2.09	-4.12	-2.09	3.50	-5.81	-3.84	-5.81
-0.40*	-2.18	-4.10	-2.18	3.60	-5.91	-3.84	-5.91
-0.30*	-2.26	-4.09	-2.26	3.70	-6.01	-3.84	-6.01
-0.20*	-2.35	-4.07	-2.35	3.80	-6.11	-3.84	-6.11
-0.10*	-2.43	-4.05	-2.43	3.90	-6.22	-3.84	-6.21
0.00	-2.52	-4.04	-2.52	4.00	-6.32	-3.84	-6.31
0.10	-2.60	-4.03	-2.60	4.10	-6.42	-3.84	-6.41
0.20	-2.69	-4.01	-2.69	4.20	-6.52	-3.84	-6.51
0.30	-2.78	-4.00	-2.78	4.30	-6.62	-3.84	-6.61
0.40	-2.86	-3.99	-2.86	4.40	-6.72	-3.85	-6.70
0.50	-2.95	-3.98	-2.95	4.50	-6.83	-3.85	-6.80
0.60	-3.04	-3.97	-3.04	4.60	-6.93	-3.85	-6.90
0.70	-3.13	-3.95	-3.13	4.70	-7.03	-3.85	-6.99
0.80	-3.22	-3.94	-3.22	4.80	-7.13	-3.86	-7.08
0.90	-3.31	-3.94	-3.31	4.90	-7.24	-3.86	-7.18
1.00	-3.40	-3.93	-3.40	5.00	-7.34	-3.86	-7.26
1.10	-3.49	-3.92	-3.49	5.10	-7.44	-3.86	-7.35
1.20	-3.59	-3.91	-3.59	5.20	-7.54	-3.87	-7.43
1.30	-3.68	-3.90	-3.68	5.30	-7.65	-3.87	-7.51
1.40	-3.77	-3.89	-3.77	5.40	-7.75	-3.87	-7.59
1.50	-3.87	-3.89	-3.87	5.50	-7.85	-3.88	-7.65
1.60	-3.96	-3.88	-3.96	5.60	-7.96	-3.88	-7.72
1.70	-4.05	-3.88	-4.05	5.70	-8.06	-3.89	-7.78
1.80	-4.15	-3.87	-4.15	5.80	-8.17	-3.89	-7.83
1.90	-4.24	-3.87	-4.24	5.90	-8.27	-3.89	-7.88
2.00	-4.34	-3.86	-4.34	6.00	-8.37	-3.90	-7.92
2.10	-4.43	-3.86	-4.43	6.10*	-8.48	-3.90	-7.96
2.20	-4.53	-3.85	-4.53	6.20*	-8.58	-3.91	-7.99
2.30	-4.63	-3.85	-4.63	6.30*	-8.69	-3.91	-8.02
2.40	-4.72	-3.85	-4.72	6.40*	-8.79	-3.91	-8.04
2.50	-4.82	-3.85	-4.82	6.50*	-8.90	-3.92	-8.06
2.60	-4.92	-3.84	-4.92	6.60*	-9.00	-3.92	-8.08
2.70	-5.02	-3.84	-5.02	6.70*	-9.10	-3.93	-8.09
2.80	-5.12	-3.84	-5.12	6.80*	-9.21	-3.93	-8.11
2.90	-5.21	-3.84	-5.21	6.90*	-9.31	-3.94	-8.12

* Values for HC5 are given over the interval of log K_{ow} = -1 to 7; 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.

APPENDIX 5: TRANSPORT ROUTES AND MAIN CHARACTERISTICS OF THE SIM- PLEBOX 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 5 (§ 3.2.2), 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	$1.4 \cdot 10^{-3}$ m/s
organic carbon content suspended matter	10%	mass transfer water side air-water interface	$1.4 \cdot 10^{-5}$ m/s
organic carbon content sediment	5%	mass transfer water side water-sed interface	$2.8 \cdot 10^{-7}$ m/s
organic carbon content soil 1	5%	mass transfer water side water-sed interface	$1.8 \cdot 10^{-7}$ m/s
organic carbon content soil 2	5%	mass transfer air side air-soil interface	$1.4 \cdot 10^{-3}$ m/s
organic carbon content soil 3	5%	mass transfer soil air side air-soil interface	$5.6 \cdot 10^{-6}$ m/s
temperature	12°C	mass transfer soil water side air-soil interface	$5.6 \cdot 10^{-10}$ m/s

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Setting Integrated Environmental Quality Standards for Substances in The Netherlands

**Environmental quality standards
for soil, water & air**

Interdepartmental Working Party on Setting Integrated Environmental Quality
Standards for Substances

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**Setting Integrated Environmental Quality Standards
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January 1999
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Interdepartmental Working Party on Setting Integrated Environmental Quality
Standards for Substances

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Foreword

Standards for the desired environmental quality are only set for a certain period at a time. This is because our scientific knowledge of the harmful effects of substances is evolving rapidly. It is desirable that new knowledge be used to evaluate existing standards, and to set standards for substances for which none have yet been established, where desirable. The existing system of environmental quality standards for water and soil, presented in the 1991 'MILBOWA' policy memorandum, is at least six years old. The present document contains a new set of standards for the next few years based on the latest knowledge, in which special attention has been paid to harmonisation with the standards for air. The text and the standards in the present document were developed in close interaction with what is presented with respect to environmental quality standards in the Fourth National Policy Document on Water Management - Government Decision and the Third National Environmental Policy Plan.

Standards are set in consultation with many interested parties. In the first place, figures are derived scientifically by the National Institute for Public Health and Environment (RIVM) in consultation with the Institute for Inland Water Management and Wastewater Treatment (RIZA), based on a number of policy principles regarding the desired degree of protection for humans and for ecosystems. The underlying scientific basis is scrutinised by the research supervisory group of the Integrated Standards for Substances project and by the Health Council and the Technical Committee on Soil Protection. An advisory body was also set up in mid-1996 to deal with policy issues, made up of representatives of employer organisations (VNO-NCW), the pressure group *Natuur en Milieu*, the Dutch Phytopharmacological Association (NEFYTO) and the Dutch Chemical Industry Association (VNCI), as well as representatives of the provinces (IPO), the municipalities (VNG) and the water boards (UvW). The comments made by these organisations on the text of this Memorandum and on the proposed standards were taken into account as far as possible.

This Memorandum was drawn up under the responsibility of the Interdepartmental Working Party on Integrated Standards for Substances, which included representatives not only of the Ministry of Housing, Spatial Planning & the Environment, but also of the Ministry of Transport, Public Works & Water Management, the Ministry of Agriculture, Nature Management & Fisheries and the Ministry of Economic Affairs.

J.F.M. van Vliet

Chairman, Interdepartmental Working Party on Setting Integrated Environmental Quality Standards for Substances

For information please contact:

Ms M. van der Weiden

Ministry of Housing, Spatial Planning and the Environment (VROM)

DGM/SVS, IPC655

P.O.Box 30945

2500 GX The Hague

Fax: +31 70 3391297

Summary

This Memorandum presents general non-legally binding environmental quality standards for soil, water and air. The standards involved are the 'maximum permissible concentration' (MPC) and the target value, and are presented for 150 substances. The standards are based on ecotoxicological criteria, and were produced as part of the Setting Integrated Environmental Quality Standards for Substances (INS) project.

The standards represent concentrations at which ecosystems are assumed to be protected. MPCs for a limited number of substances (volatile compounds) in air were derived explicitly with a view to protecting human health because it was estimated that these substances pose greater risks to humans than to other organisms.

The MPC is the concentration of a substance, derived scientifically, at which no adverse effect is expected or, in the case of carcinogenic substances, a probability of fatality of 10^{-6} can be predicted. In deriving the MPC and target value, no account is taken of economic considerations. Such considerations should be taken into account when the standards are translated into targets with respect to source-oriented measures, i.e. to reduce emissions of substances. The target value is the concentration at which the environmental impact is expected to be negligible. The MPC and the target value place an obligation on decision-makers to make efforts to comply with the standards. The NEPP3 refers to this document and stipulates that the goal of policy is to ensure that, in the short term, if possible by 2000, the MPC for all substances must no longer be exceeded as a result of emissions, and that in the longer term, if possible by 2010, the target value must no longer be exceeded due to emissions.

Amongst the main applications of environmental quality standards are the assessment of environmental quality and the evaluation of the effectiveness of pollution abatement policy. This Memorandum examines the use of the standards to assess environmental quality in the various environmental media. The standards come into force when they are incorporated into specific policy documents such as the Fourth National Policy Document on Water Management.

In 1991, standards for soil and water were presented for over 100 substances in the policy statement on the MILBOWA Memorandum (Second Chamber, 1991-1992). The standards for 30 of these substances were based for the first time on risk assessment. These risk assessments, and therefore the standards, have now been revised. A risk assessment has been carried out for the first time for some further 120 substances. The MILBOWA Memorandum also included standards for a number of specific environmental substances such as nutrients, oxygen and chloride that were not based on risk assessment. These standards are also included unchanged in this document.

This Memorandum supersedes all the MILBOWA standards. The approximately 150 new standards will remain in force for about five years, after which the desirability of a re-assessment will be considered. Only standards which prove to be incorrect in the light of new scientific evidence will be revised before then.

The approach proposed in this Memorandum differs in a number of respects from that in the MILBOWA Memorandum. The term 'limit value', used in MILBOWA, is now reserved for

legally binding standards. Furthermore the MILBOWA Memorandum confined itself to standards for soil and water. This Memorandum presents standards for soil, water and air which have been harmonised such that the standard for a given environmental medium also provides protection to organisms in other media. Where relevant, in standard setting allowance is made for secondary poisoning, the phenomenon by which persistent, toxic compounds accumulate in higher organisms such as birds and mammals, through the food chain. In deriving standards for metals, allowance was also made for the natural background concentrations of these substances.

1 Introduction

Policy with regard to polluting substances is directed towards achieving a healthy and clean environment. It takes the form of a source-oriented approach aimed at preventing unnecessary pollution. Environmental quality standards are an important tool in determining the need for and the success of this approach. These standards provide a benchmark for the assessment of environmental quality data, and can also be used in setting priorities. Standards were first formulated for air and water in the 1970s, and for soil in the early 1980s.

The purpose of this Memorandum is to present environmental quality standards for 150 substances, based on risk assessments. Furthermore, the standards for the different environmental media have been harmonised. The Memorandum also indicates how the standards can be applied.

Over the years, environmental quality standards have been modified on several occasions to reflect developments in our understanding and approach. The 1991 policy statement on the 'MILBOWA' Memorandum¹ took stock of the previous environmental quality standards for soil and water. This Memorandum presented environmental quality standards² for soil and water for more than 100 substances. Only about 30 of these were based on a risk assessment.

Since then, environmental quality standards based on a risk assessment approach have been formulated for many more substances under the INS (Setting Integrated Environmental Quality Standards for Substances) project. Standards were drawn up not only for soil and water but also, where possible, for air. The standards previously established in MILBOWA on the basis of risk assessment were also critically re-evaluated. The results of the INS project are presented in this document. Most of the existing standards for soil and water have been revised either upwards or downwards. For air, only six new MPCs and target values have been formulated.

This Memorandum supersedes all the MILBOWA standards. The standards now presented will remain in force for about five years, after which the possibility of a re-assessment will be considered. Only standards which prove to be manifestly incorrect will be revised before then. In the case of pesticides, there is a special, ongoing procedure for reviewing standards based on the pesticides approval procedure. A working party of the Dutch Health Council has drawn up recommendations on zinc and on a risk assessment methodology for essential elements. These recommendations have been brought in into the EU risk assessment with respect to zinc being carried out in the framework of the EU-Regulation for existing substances (Regulation 1488/94). In case the results of the EU-risk assessment, which are

¹ The MILBOWA Memorandum (Second Chamber 1990-1991, 21990 no. 1) set out the proposed standards. A policy statement was issued in response to the Memorandum, which contained the standards as formally adopted by the Second Chamber (Second Chamber 1991-1992, 21990 and 21250, no. 3). For purposes of brevity the term 'MILBOWA' will be used here to refer to the policy statement.

² The MILBOWA used the term 'environmental quality objectives'. We now speak of 'environmental quality standards'. The difference between these terms is indicated in the National Environmental Policy Plan 3.

expected by the end of 1999, give arguments to change the MPC and target value for zinc, the values will be adjusted.

Desirability of an integrated approach to standard-setting

An integrated approach to standards across the environmental media offers certain advantages. The main advantage is that account is taken of transfers between the different media. Polycyclic aromatic hydrocarbons (PAH), for example, are emitted into the atmosphere from combustion processes, but may eventually end up in sediments via water. Allowance has been made wherever possible for inter-media relationships of this kind. The intention was to ensure that the standards set for a given medium also provide protection for the other media. In the case of the standards for air, this was only possible to a limited extent because of gaps in our knowledge.

Another advantage of an integrated approach is that it allows the terminology and practical application to be standardised. This helps to make environmental policy more transparent. Inconsistencies which have developed in the past can be reduced. This does, however, not mean that standard-setting for the different media becomes completely comparable. The nature of the media are too different for this. The transient nature of air pollution, for example, demands a different approach from that needed for the often immobile contaminants in the soil.

The substances concerned

The MILBOWA contained environmental quality standards based on risk assessment for heavy metals, polycyclic aromatic hydrocarbons (PAH), chlorophenols and pesticides. Most of these substances are so-called priority substances. The MILBOWA also listed some 100 other existing standards. The present document extends the number of standards based on risk assessment by eight metals, some 45 volatile compounds and some 70 pesticides. These substances were selected when the INS project started around 1990 because, for example, they featured on national and international lists. The total number of substances involved is about 150. Risk assessments had been carried out within MILBOWA for about 30 of these substances. It was decided that the existing standards for a number of substances set at the level of the detection threshold, could be dropped. As far as is known these substances do not present problems.

The MILBOWA also included the standards applying to soil, groundwater and surface waters for nutrients, eutrophication parameters, the so-called general parameters (e.g. oxygen, pH), salts, radiological parameters and bacteriological parameters. These standards are also included unchanged in this document. Possible changes in the standards for nutrients will be announced around 2000 when the Integrated Memorandum on Manure and Ammonia is evaluated.

Toxicological risk limits: basis for standard setting

The toxicity of substances is expressed, for the purposes of standard setting, in terms of toxicological risk limits as defined in the third National Environmental Policy Plan (NEPP3). Two such toxicological risk limits are distinguished: the 'maximum permissible concentration' (MPC) and the 'negligible concentration' (NC). These toxicological risk limits are defined in chapter 2. The concentrations of substances corresponding to these risk levels

have been calculated by the RIVM (National Institute of Public Health and Environmental Protection), and form the basis of the standards.

Types of standards and their status

The NEPP3 distinguishes the following types of standards:

Legally binding

- limit value: a standard which must be observed;
- guideline value: a standard which must be taken into account.

Non-legally binding

- Maximum permissible concentration (MPC): the concentration, derived scientifically, at which no adverse effect is expected (human and ecosystem protection), or for which a probability of fatality of 10^{-6} or less can be predicted (with respect to human protection only)
- Target value: the concentration at which the environmental effects are negligible.

This document presents only non-legally binding standards, i.e. MPCs and target values. The relevant authorities are required to make efforts to meet these standards. The NEPP3 stipulates that, within the very short term and if possible by 2000, the MPC must no longer be exceeded as a result of emissions, and that in the longer term, if possible by 2010, the target value must no longer be exceeded as a result of emissions. The MPC and target values can therefore be used as a benchmark to assess the results of environmental policy and as a tool for prioritising policy on emissions. General principles of environmental policy such as the precautionary principle and the standstill principle will continue to apply.

As indicated above, no hard and fast timetable has been adopted for achieving the MPCs (or the target values). The values contained in this document will therefore only become operative or have an impact, for example on source oriented emission targets for particular target groups, when they are adopted in specific policy documents. The values of the standards contained in this document were adopted in the Fourth National Policy Document on Water Management - Government Decision (NW4 - Regeringsbeslissing, to be published early 1999) as minimum water quality standards (MPC) and target values. The Policy Document indicate the importance of MPCs and target values as an instrument of water policy.

Changes have been made to the system of standards presented in the MILBOWA (1991). One important change is that the terms 'limit value' and 'guideline value' will henceforth be reserved for legally binding standards. Only non-legally binding standards are dealt with in the present document. The limit values in MILBOWA which were not legally binding are abrogated and now being replaced by MPCs. MPCs differ in several respects from MILBOWA limit values. MPCs (and target values) take no account of economic considerations and realizability, for example. Such considerations should be taken into account when the standards are translated into targets with respect to source-oriented measures, i.e. to reduce emissions of substances.

Advisory reports

MPCs and NCs for substances are published in RIVM reports. Recommendations on the risk assessment methodology used in general were requested from the Health Council and the Technical Committee on Soil Protection. An additional request for an advisory report on zinc was dealt with by the Health Council. The MPCs and target values in this document were drawn up on the basis of these recommendations and a number of technical choices. The manner in which they were dealt with, and the choices made, are described in this Memorandum. Differences in the nature of environmental problems in the different environmental media, and the interface with other policy areas and with international activities were also taken into account. The discussions held with the regional and local authorities and the target groups on the proposed environmental quality standards also played an important role.

International harmonisation

It is important that procedures for setting environmental quality standards should be harmonised at the international level. Water and air do not respect national frontiers. Furthermore, excessive differences between countries are undesirable in terms of fair competition. There is already close cooperation, particularly when it comes to scientific methods for deriving standards. In Europe, for example, risk assessments for both new and existing substances (including the EU priority substances) must be performed in accordance with principles laid down in community legislation (Council Directive 93/67/EEC and Regulation 1488/94 respectively). The risk assessment methodology is specified in greater detail in the EU Technical Guidance Documents. The WHO has produced Air Quality Guidelines based on toxicological criteria for priority air pollutants. The European Union is using them in drawing up the standards for its framework directive on air quality.

As far as water is concerned the main European developments are the drawing up of environmental criteria for pesticide approval and the derivation of water quality standards within the framework of the EU Water Framework Directive (EU Commission's proposal for a Council Directive establishing a framework for a Community action in the field of water policy). It is expected that the environmental quality standards presented in the underlying document closely relate to the "good surface water status" as referred to in Annex V of the Water Framework Directive. Furthermore, the international forum in which standards for water are set are determined on sea or river basin conventions. The countries bordering the Rhine have set targets for the Rhine. The countries bordering the North East Atlantic have prepared standards (ecotoxicological assessment criteria) for the marine environment within the OSPARCOM (Oslo and Paris Commission).

The EU-project 'CARACAS' (Concerted Action on Risk Assessment for Contaminated Sites in the European Union) is intended to improve the coordination between European countries with respect to the science underlying the assessment of the risks of contaminated soil.

Despite this international coordination, there are differences in standard setting between countries. National standards are important, partly because there are many substances for which there are as yet no international toxicological assessments, and partly because the system for setting standards in a particular country will be consistent with its regulatory regime, and reflect the nature and magnitude of its environmental problems.

New developments

Standards do not remain static. The methodology used and the theory underlying effect-based environmental quality standards are evolving continuously. Issues such as bio-accumulation (of PCBs for example), standards based on bio-availability, hormone disruption effects and how essential elements should be dealt with require constant attention. As indicated above, the standards here presented will remain in force for at least five years, and will only be modified in the meantime if one of the standards proves, on the basis of new information, to be manifestly incorrect.

Aspects not covered by this memorandum

There are a number of misconceptions about standards, and these could produce false expectations in regard to this memorandum. This memorandum does not deal, for example, with the standards for the clean-up of contaminated soil. There is a separate framework of standards - the soil clean-up intervention values - for this. It also does not cover policy on the disposal of dredging spoil and the standards and criteria used in this connection. This means that for the time being the existing limit value will be maintained as the criterion for the classification of dredging spoil. Nor is this Memorandum intended to set standards for specific purposes, functions or products, e.g. standards for drinking water quality or swimming water. The familiar, function-oriented standard (of 0.1 µg/l) for pesticides in groundwater used for the preparation of drinking water is therefore not included in this document. This Memorandum contains general environmental quality standards applying throughout the Netherlands, and not standards applying to specific areas or regions.

Structure of this Memorandum

Chapter 2 explains how the scientific toxicological risk limits (MPC and NC) were derived. Chapter 3 presents the standards and describes the decisions taken in setting them. Chapter 4 explains how the standards should be used.

2 Scientific derivation of toxicological risk limits: MPC and NC

This chapter considers the scientific derivation of the maximum permissible concentration (MPC) and the negligible concentration (NC). These toxicological risk limits constitute the basis for the determination of environmental quality standards (see Ministry of Housing, Spatial Planning and the Environment: Dealing with Risks, 1989), and are calculated by the RIVM (National Institute for Public Health and the Environment).

MPC

The MPC is defined, for the purposes of policy on dangerous substances, as the concentration of a particular substance in a particular environmental medium for which:

- 1 no adverse effect on ecosystems is expected,
- 2a (for non-carcinogenic substances) no adverse effects on human health are expected, or
- 2b (for carcinogenic substances) the probability of mortality for a person does not exceed 10^{-6} per year.

The MPC is determined *per substance*. As far as effects on ecosystems are concerned, the intention is to protect the species in that ecosystem. The ecosystem itself is then assumed to be protected.

NC

The NC is the lower risk threshold for a substance, and is in principle set at 1/100 of the MPC. The purpose of the reduction by a factor of 100 is to reflect the fact that many pollutants actually occur together in the environment. The reduction makes an allowance for their combined toxicity. Although it would probably be desirable to incorporate some differentiation into the reduction (for example by substance group and/or environmental circumstances) rather than use a constant value of 100, the fixed factor of 100 has been retained, based on the advice of the Health Council and the Technical Committee on Soil Protection.

Content of advisory reports

As mentioned in the introduction, an evaluation was made of the MPCs and NCs calculated in 1991 for 30 substances in connection with the MILBOWA Memorandum. New MPCs and NCs have also been calculated for some further 120 substances.

Consideration was given, within the INS project, to advices on the MILBOWA Memorandum submitted by a variety of organisations (e.g. the Health Council, the Technical Committee on Soil Protection, the environmental pressure group *Natuur en Milieu* and the Committee for Integrated Water Management).

The policy statement issued in response to the MILBOWA Memorandum included the main recommendations made by these organisations, i.e.:

- the toxicological risk limits for water and soil should be harmonised with those for air,
- account should be taken of naturally occurring background concentrations of metals in the water and soil in setting MPCs and NCs,
- allowance should be made for secondary poisoning. Secondary poisoning is the phenomenon by which persistent, toxic compounds accumulate in higher organisms

(birds, mammals) through the food chain (fish, mussels, earthworms). This leads to higher organisms at the top of the food chain being particularly exposed to these compounds.

All three of these points are dealt with in this chapter.

After a substantial number of the MPCs and NCs had been calculated, the Health Council and the Technical Committee on Soil Protection were again asked to prepare an advisory report on the data and methodologies being used. Both of these bodies indicated that the toxicological risk limits provided a good picture reflecting current knowledge, but also pointed out that there were major uncertainties in some cases, relating to the methods used and the lack of toxicity data. Both bodies made recommendations on long-term research into how uncertainties resulting from the methods used can be reduced. Research has now begun in response to this advice, and is expected to produce results which can be used in a later evaluation.

Derivation of MPCs and NCs

All the MPCs were calculated by the RIVM from published (eco)toxicological data. These were reported by substance group (see References). In the case of pesticides, use was made both of published ecotoxicological data and of data from the dossiers compiled in connection with the pesticides approval procedure. If so-called no-effect concentrations are available for four or more different taxonomic groups of organisms with prolonged exposure, an MPC for the relevant environmental medium is estimated by means of a statistical extrapolation procedure. If no more than three values are available, the MPC is instead determined by using fixed safety factors. Where there are very few toxicity data, an additional safety factor of 10 is applied.

For a limited number of substances (volatile compounds) MPCs for air were derived specifically on the basis of human health considerations. Human exposure via the atmosphere is judged to be the critical risk in setting these standards.

Separate MPCs are set for each environmental medium. Because there are naturally occurring transfers between the media, the MPCs for the different media are then harmonised, using the principle that the risk limit in one medium should not be such as to lead to the risk limit in another medium being exceeded. This means that the MPC used for one environmental medium also provides protection for organisms in the other media.

There are often no toxicity data available for sediments. The MPC for sediments is therefore calculated from the MPC for surface water. If there are no data for the terrestrial environment, the MPC for the soil is also calculated from the scientifically determined MPCs for surface water. In the absence of ecotoxicological data for groundwater the MPC and NC for groundwater are set equal to the MPC and NC for surface water.

Adequate toxicological data for air exist in only a limited number of cases. Inter-medium harmonisation of MPCs and NCs was only possible for six volatile compounds. As indicated above, these were based explicitly on human health criteria because human exposure via the atmosphere is considered the critical risk. For many substances, however, the ecotoxicological data needed to calculate MPCs for air in the same way as for soil and water

do not exist. These are generally substances for which there is no pre-existing reason to expect the standard to be determined by the risk to human health. It is the case, however, that air transport can be an important component of the environmental pathways of these substances (for example via atmospheric deposition to water or soil).

Toxicological risk limits for metals

In determining standards for metals, account needs to be taken of the fact that they also occur naturally in the environment. This is done by adopting an 'added risk' approach. This means that the toxicological risk limits calculated are regarded as applying to anthropogenic additions, and are added to naturally occurring concentrations. Any possible effects on ecosystems due to naturally occurring metals are not regarded as adverse, but as contributing to the natural diversity of ecosystems.

In calculating the MPCs and NCs, allowance was made when choosing the toxicity data for the fact that some metals are essential to biological processes. As far as can be determined from the data available, the standards presented in this document fall outside the range within which the concentrations restrict the functioning of organisms.

No allowance was made, in deriving the MPCs and NCs, for chemical, biological and physical parameters such as hardness or pH, because they are of subsidiary importance or because not enough is known about these factors to permit their effect to be quantified.

Given the fact that zinc is an essential element a working party of the Dutch Health Council has drawn up recommendations on zinc and on a risk assessment methodology for essential elements. These recommendations have been brought in into the EU risk assessment with respect to zinc being carried out in the framework of the EU-Regulation for existing substances (Regulation 1488/94). In case the results of the EU-risk assessment, which are expected by the end of 1999, give arguments to change the MPC and target value for zinc (and other essential elements), these values will be adjusted.

Secondary poisoning

All 150 substances were checked for their tendency for secondary poisoning. Secondary poisoning is the phenomenon by which persistent, toxic compounds accumulate along the food chain so that higher organisms (birds, mammals) undergo increased exposure, and eventually suffer adverse effects. Calculations were made for those substances which may show secondary poisoning, using simplified food chains (aquatic and terrestrial) and toxicity data for birds and mammals, to determine whether secondary poisoning constitutes a critical exposure pathway. Where this is the case, appropriate allowance was made for this in calculating the MPC. In the case of metals, this evaluation did not lead to modification of the MPCs.

There are several ways of allowing for the risks associated with secondary poisoning. The two main methods have been described by the RIVM. In one method, separate toxicological risk limits are calculated to reflect the toxic effects on higher organisms (secondary poisoning). These toxicological risk limits are then compared with toxicological risk limits based on direct effects on the other organisms in an ecosystem, and the lower of the two values is adopted. In the other method a single-stage determination of the critical concentration is made, based on the combination of the indirect effects (secondary poisoning)

and the direct effects on all the organisms in an ecosystem. The Technical Committee on Soil Protection and the Health Council were asked to produce advisory reports on these methods. The conclusions of the two bodies differed, and the second method was eventually adopted, in line with the advice of the Technical Committee on Soil Protection. An important argument was that this method is more consistent with the principle that standards should be such as to protect an ecosystem as a whole rather than the separate components of the ecosystem.

3 Formulation of environmental quality standards

The previous chapter explained how toxicological risk limits, harmonised between the different media, are derived. These toxicological risk limits form the basis on which the environmental quality standards MPC and target value are set.

MPC and target value

The following general principles apply to the setting of MPCs and target values:

- the MPC and the target value are in principle based on the toxicological risk limits calculated by the RIVM;
- the values are harmonised with standards set in other frameworks (e.g. international agencies, pesticide approval policy, soil clean-up intervention values);
- in the case of naturally occurring substances, the MPC and the target value are based on the sum of the background concentration in the Netherlands and the maximum permissible and negligible (ecotoxicological) risk limit respectively. The background level is taken as the upper limit of the concentrations measured in relatively unpolluted areas.

This memorandum sets MPCs and target values for the aquatic medium (surface water and sediments), the terrestrial medium (soil and groundwater) and air. Both environmental quality standards are not necessarily set for each environmental medium. Furthermore, standards are not set for substances unlikely to be a problem in a particular medium. The MPCs and target values are shown in table 1.

Terrestrial medium: soil and groundwater

The terrestrial medium includes both soil and groundwater.

Policy for the soil makes use of target and intervention values. Because soil quality changes only very gradually, there is considered to be no point in supplementing these values by short-term standards in the form of MPCs. MPCs as derived in the INS project and published in RIVM reports are therefore not relevant in soil policy.

The target values for soil and sediment are based on the most critical NC for soil or sediment. This means that changes of circumstances resulting, for example, by dredging up sediments, land reclamation and inundation do not cause standards to be exceeded.

The NCs for surface water were used to determine the target values for groundwater. There is a lack of toxicity data for groundwater organisms. Because such organisms are exposed via the water phase, it is assumed that the NCs for surface water also provide a good estimate of toxicity for groundwater organisms. These values were compared with the intervention values for groundwater. In some cases the intervention values were lower. The main reason for this is that they are based partly on a specific human toxicology risk assessment. In such situations, the target values for groundwater are set at the current intervention values. If the intervention values are revised, this may affect the target values. Table 1 indicates the substances concerned. The target values for groundwater are given in terms of concentrations of dissolved components.

Aquatic medium: surface water and sediments

In the aquatic medium, MPCs and target values have been formulated for surface water and sediment. In the case of surface water, figures have been given for both the dissolved component and in total. The figures for water-total are calculated from those for the dissolved component, and relate to standard water with 30 mg/l suspended solids. MPCs and target values for sediments relate to sediments with a standard composition.

In deriving the MPCs the toxicity data collected were supplemented with data used in deriving the recent targets (Zielvorgaben) for the International Commission for the Protection of the Rhine, on the condition that these data met the RIVM quality criteria.

The MPCs for sediments were derived from the MPCs for surface water using substance specific equilibrium partition coefficients. Where the MPCs thus calculated came out higher than the current intervention values for contaminated soil/sediments, they were set at the intervention values. If the intervention values are revised, this may affect the MPCs. As already mentioned, the target values for sediments and soil were set at the same level, based on the more critical of the two NCs (soil or sediment).

It was concluded, on the basis of the toxicity data available, that freshwater and salt water organisms are equally sensitive to pollutants. The standards, which were derived from the combined toxicity data for both fresh and salt water, therefore also apply to both freshwater and marine systems. This does not apply to organotin compounds, however. Salt water organisms appear to be more sensitive to organotin compounds than freshwater organisms, and separate standards have therefore been set for fresh and salt water.

Air

MPCs and NCs for air were only set for substances which, because of their volatility, may present a threat to human health. This was limited to substances for which RIVM had sufficient toxicity data to derive reliable toxicological risk limits. For many substances sufficient the required minimum set of data was not available. The resulting toxicological risk limits were then compared with recent air quality data. This showed that only a limited number of substances are expected to exceed their NC, mainly those included on the priority substances list. This Memorandum contains target values for a few substances for which standards had not yet been set and which can potentially exceed their NC. The harmonisation of already existing air quality standards with risk limits for soil and water did not necessitate any adjustments to the existing air quality standards.

Tabel 1: ENVIRONMENTAL QUALITY STANDARDS FOR SOIL, WATER AND AIR

The values for water-total apply to the standard containing 30 mg/l suspended solids;
the values for soil and sediment apply to the standard soil (s.s.) containing 10 % organic matter and 25 % lutum.
For conversion of measured values to values applying to standard water-total and/or standard-soil, see Annex 2
With respect to air only new established values are included in the table.

METALS	SURFACE WATER (dissolved)			SURFACE WATER (water-total)			SEDIMENT & SOIL (dry matter)		SEDIMENT (dry matter)		GROUND WATER (dissolved)	
	general		MPC (incl. BC)	general		MPC (incl. BC)	general		MPC-sed (incl. BC)		general	
	background concentrat (BC)	target value (incl. BC)		background concentrat (BC)	target value (incl. BC)		background concentrat (BC)	target value (incl. BC)	background concentrat (incl. BC)		background concentrat (BC)	target value (incl. BC)
	µg/l	µg/l	µg/l	µg/l	µg/l	µg/l	mg/kg s.s.	mg/kg s.s.	mg/kg s.s.	mg/kg s.s.	µg/l	µg/l
cadmium	0.08	0.08	0.4	0.4	0.4	2	0.8	0.8	12 #	0.06	0.06	0.06
mercury (inorganic)	0.01	0.01	0.2	0.06	0.07	1.2	0.3	0.3	10 #	-	-	0.01
methyl-mercury	0.01	0.01	0.02	0.06	0.06	0.1	0.3	0.3	1.4	-	-	0.01
copper	0.4	0.5	1.5	1.1	1.1	3.8	36	36	73	1.3	1.3	1.3
nickel	3.3	3.3	5.1	4.1	4.1	6.3	35	35	44	2.1	2.1	2.1
lead	0.2	0.3	11	3.1	5.3	220	85	85	530 #	1.6	1.6	1.7
zinc	2.8	2.9	9.4	12	12	40	140	140	620	24	24	24
chromium	0.2	0.3	8.7	1.6	2.4	84	100	100	380 #	2.4	2.5	2.5
arsenic	0.8	1	25	1	1.3	32	29	29	55 #	7	7.2	7.2
antimony	0.3	0.4	6.6	0.3	0.4	7.2	3	3	15 #	0.09	0.15	0.15
barium	73	76	220	76	78	230	160	160	300	200	200	200
beryllium	0.02*	0.02*	0.2	0.02*	0.02*	0.2	1.1	1.1	1.2	0.05*	0.05*	0.05*
cobalt	0.2*	0.2*	2.8	0.2*	0.2*	3.1	9	9	19	0.6*	0.7*	0.7*
molybdenum	1.4	4.3	290	1.4	4.4	300	0.5	3	200 #	0.7	3.6	3.6
selenium	0.04	0.09	5.3	0.04	0.09	5.4	0.7	0.7	2.9	0.02	0.07	0.07
thallium	0.04*	0.06*	1.6	0.04*	0.06*	1.7	1	1	2.6	<2*	2*	2*
tin	0.0002*	0.2	18	0.002*	2.2	220	19	-	-	<2*	<2*	2.2*
vanadium	0.8*	0.9*	4.3	1	1	5.1	42	42	56	1.2	1.2	1.2

ORGANIC SUBSTANCES	SURFACE WATER			SEDIMENT & SOIL		GROUND WATER		AIR	
	MPC (dissolved)	target value (water-total)	MPC (water-total)	target value (dry matter)	MPC-sed (dry matter)	target value (dissolved)	target value	target value	MPC
PAHs	<u>µg/l</u>	<u>µg/l</u>	<u>µg/l</u>	<u>mg/kg s.s.</u>	<u>mg/kg s.s.</u>	<u>µg/l</u>	<u>µg/m³</u>	<u>µg/m³</u>	<u>µg/m³</u>
naphthalene	1.2	0.01	1.2	0.001*	0.1	0.01			
anthracene	0.07	0.0008*	0.08	0.001*	0.1	0.0007*			
phenanthrene	0.3	0.003*	0.3	0.005*	0.5	0.003*			
fluoranthene	0.3	0.005	0.5	0.03	3	0.003			
benzo(a)anthracene	0.01*	0.0003*	0.03*	0.003*	0.4	0.0001*			
chrysene	0.3	0.009*	0.9	0.1	11	0.003*			
benzo(k)fluoranthene	0.04	0.002*	0.2	0.02	2	0.0004*			
benzo(a)pyrene	0.05	0.002*	0.2	0.003*	3	0.0005*			
benzo(ghi)perylene	0.03	0.005	0.5	0.08	8	0.0003			
Indeno(123-cd)pyrene	0.04	0.004*	0.4	0.06	6	0.0004*			
sum 10-PAHs				1***					
volatile halogenated hydrocarbons	<u>µg/l</u>	<u>µg/l</u>	<u>µg/l</u>	<u>mg/kg s.s.</u>	<u>mg/kg s.s.</u>	<u>µg/l</u>	<u>µg/m³</u>	<u>µg/m³</u>	<u>µg/m³</u>
monochlorobenzene	690	7	690	0.08	8	7			
dichlorobenzenes(Ind)	250	3	250	0.004	6	3			
trichlorobenzenes(Ind)	67	0.7	67	0.002	7	0.7			
tetrachlorobenzenes(Ind)	24	0.2	24	0.007	7	0.2			
pentachlorobenzene	0.3	0.003	0.3	0.001	0.1	0.003			
hexachlorobenzene	0.009	0.00009*	0.009	0.0005	0.005	0.00009*			
benzene	240	2	240	0.01*	1	2			
acrylonitril	81	0.081	81	0.000007*1	0.0007*1	0.081			
3-chloropropene	3	0.03*	3	0.00005	0.005	0.03*		0.07	7
dichloroethanes(Ind)	700	7	700	0.02*	2	7			
1,1-dichloroethene	3400	34	3400	0.1*	12	34		2	200
1,2-dichloroethene	6100	61	6100	0.2	1 #	20 #			
dichloromethane	20000	200	20000	0.4	20 #	200			
1,2-dichloropropane	76	0.8	76	0.002*	0.2	0.8			
1,3-dichloropropane	76	0.8	76	0.002*	0.2	0.8			
1,3-dichloropropene	8	0.08	8	0.0002*	0.02*	0.08		250~	25000~
2,3-dichloropropene	8	0.08	8	0.0004*	0.04*	0.08		0.1	12
ethene	8500*	85*	8500*	0.06	6	85*		0.4	40
ethylbenzene	370	4	370	0.03	3	4			
ethylenoxide	84*1	0.8*1	84*1	0.000021	0.0021	0.8*1			
hexachloroethane	83	0.8	83	0.2	17	0.8			
monochlorotoluenes(Ind)	310*	3*	310*	0.3	33	3*			
pentachloroethane	230	2	230	0.5	49	2			
styrene	570	6	570	0.3	25	6			

ORGANIC SUBSTANCES (continued)	SURFACE WATER			SEDIMENT & SOIL		GROUND WATER		AIR	
	MPG (dissolved)	target value (water-total)	MPG (water-total)	target value (dry matter)	MPG-sed (dry matter)	target value (dissolved)	target- value		
	<u>µg/l</u>	<u>µg/l</u>	<u>µg/l</u>	<u>mg/kg s.s.</u>	<u>mg/kg s.s.</u>	<u>µg/l</u>	<u>µg/m³</u>	<u>µg/m³</u>	<u>µg/m³</u>
1.1.2.2-tetrachloroethane	3300	33	3300	0.1	14	33			
tetrachloroethene	330	3	330	0.002	4	3	2.5		250
tetrachloromethane	1100	11	1100	0.4	1 #	10 #			
toluene	730	7	730	0.01	4	7			
1.1.1-trichloroethane	2100	21	2100	0.07	7	21			
1.1.2-trichloroethane	7900	79	7900	0.4	39	79			
trichloroethene	2400	24	2400	0.1	13	24			
trichloromethane	590	6	590	0.02	2	6			
vinylchloride	820	8	820	0.01	0.1 #	0.7 #			
xylene (Ind)	380	4	380	0.1	14	4	48		4800
chlorophenols									
monochlorophenols(Ind)	<u>µg/l</u>	<u>µg/l</u>	<u>µg/l</u>	<u>mg/kg s.s.</u>	<u>mg/kg s.s.</u>	<u>µg/l</u>			
26	26	0.3	25	0.002	0.2	0.3			
dichlorophenols(Ind)	15	0.2	15	0.003	0.3	0.2			
trichlorophenols(Ind)	3	0.03*	3	0.001	0.1	0.03*			
tetrachlorophenols(Ind)	1	0.01*	1	0.001	0.3	0.01*			
pentachlorophenol	4	0.04*	4	0.002	0.3	0.04*			
chlorinated organics									
aldrin	<u>ng/l</u>	<u>ng/l</u>	<u>ng/l</u>	<u>µg/kg s.s.</u>	<u>µg/kg s.s.</u>	<u>ng/l</u>			
0.9*	0.9*	0.01*	1	0.06*	6	0.009*			
dieldrin	12	0.4*	39	0.5*	450	0.1			
endrin	4	0.04*	4	0.04*	4	0.04*			
DDT	0.4*	0.009*	0.9*	0.09*	9	0.004*			
DDD	0.4*	0.005*	0.5*	0.02*	2	0.004*			
DDE	0.4*	0.004*	0.4*	0.01*	1	0.004*			
α-endosulphan	20	0.2*	20	0.01*	1	0.2*			
α-HCH	3300	33	3300	3	290	33			
β-HCH	800	9	860	9	920	8			
γ-HCH (lindane)	910	9	920	0.05	230	9			
heptachlor	0.5*	0.005*	0.5*	0.007*	0.65	0.005*			
heptachloropoxide	0.5*	0.005*	0.5*	0.0002*	0.02*	0.005*			
chlordane	2*	0.02*	2*	0.03*	3*	0.02*			

ORGANIC SUBSTANCES (dissolved)	SURFACE WATER		SEDIMENT & SOIL		SEDIMENT		GROUND WATER
	MPG (dissolved)	target value (water-total)	target value (water-total)	MPC (water-total)	target value (dry matter)	MPC-seed (dry matter)	
<u>organophosphorus compounds</u>	ng/l	ng/l	ng/l	ng/l	µg/kg s.s.	µg/kg s.s.	ng/l
azinphos-ethyl	11	0.1*	0.1*	11	0.005*	0.5*	0.1*
azinphos-methyl	12	0.1*	0.1*	12	0.009*	0.9*	0.1*
chlorfenvinphos	2*	0.02*	0.02*	2*	0.0006*	0.06	0.02*
chlorpyrifos	3*	0.03*	0.03*	3*	0.01*	1	0.03*
coumaphos	0.7*	0.007*	0.007*	0.7*	0.0006*	0.06	0.007*
demeton	140	1*	1*	140	-	-	1*
diazinon**	37	0.4*	0.4*	37	0.01*	1	0.4*
dichlorvos**	0.7*	0.007*	0.007*	0.7*	0.00003*	0.003*	0.007*
dimethoate	23000	230	230	23000	0.8*	78	230
disulfoton	82	0.8*	0.8*	82	0.03*	6	0.8*
ethoprophos	63	0.6*	0.6*	63	0.003*	0.3	0.6*
fenitrothion	9*	0.09*	0.09*	9*	0.007*	0.7*	0.09*
fenthion	3*	0.03*	0.03*	3*	0.004*	0.4	0.03*
foxlm	82*1	0.8*1	0.8*1	82*1	0.08*1	81	0.8*1
heptenofos	20	0.2*	0.2*	20	0.003*	0.3	0.2*
malathion	13	0.1*	0.1*	13	0.009*	0.9	0.1*
mevinfos**	2*	0.02*	0.02*	2*	0.0006*	0.06	0.02*
oxydemeton-methyl**	35*1	0.4*1	0.4*1	35*1	0.0003*1	0.031	0.4*1
parathion(-ethyl)	2*	0.02*	0.02*	2*	0.001*	0.1*	0.02*
parathion-methyl	11	0.1*	0.1*	11	0.01*	1	0.1*
pyrazofos	40	0.4*	0.4*	40	0.02*	2	0.4*
tolclofos-methyl	7801	8*1	8*1	8001	11	1301	8*1
triazophos	32	0.3*	0.3*	32	0.007*	0.7*	0.3*
trichlorfon**	1*	0.01*	0.01*	1*	0.00002*	0.002*	0.01*
<u>organotin compounds</u>	ng/l	ng/l	ng/l	ng/l	µg/kg s.s.	µg/kg s.s.	ng/l
tetrabutyltins (ind)	16001	161	161	16001	0.8*1	781	161
salt water:	171	0.2*1	0.2*1	171	0.008*1	0.8*1	-
tributyltins (ind)**	14	0.1*	0.1*	14	0.003*	10*	0.1*
salt water:	1	0.01*	0.01*	1	0.007*	0.7*	-
triphenyltins (ind)	5	0.05*	0.05*	5	0.02*	6*	0.05*
salt water:	0.8*	0.009*	0.009*	0.9*	0.01*	1*	-

ORGANIC SUBSTANCES (continued)	SURFACE WATER			SEDIMENT & SOIL		SEDIMENT MPC-sed (dry matter)	SEDIMENT target value (dry matter)	GROUND WATER target value (dissolved)
	MPC (dissolved)	target value (water-total)	MPC (water-total)	target value	MPC-sed (dry matter)			
<u>acids</u>		<u>µg/l</u>	<u>µg/l</u>	<u>µg/kg s.s.</u>	<u>µg/kg s.s.</u>	<u>µg/l</u>		
benlazone**	64l	0.6l	64l	1l	130l	0.6l		
2,4-D	10	0.1	10	0.3*	27	0.1		
dichlorprop	40	0.4	40	32	3200	0.4		
dinoseb	0.03	0.0003*	0.03	0.003*	0.3	0.0003*		
dinoterb	0.03	0.0003*	0.03	0.1*	11	0.0003*		
DNOC	21	0.2	21	0.7	280	0.2		
MCPA	2	0.02	2	0.06*	6	0.02		
mecoprop	4	0.04*	4	0.02*	2	0.04*		
2,4,5-T	9l	0.09l	9l	0.2*	50l	0.09l		
<u>carbamates & dithiocarbamates</u>		<u>ng/l</u>	<u>ng/l</u>	<u>µg/kg s.s.</u>	<u>µg/kg s.s.</u>	<u>ng/l</u>		
aldicarb	98	1*	98	0.001*	0.1	1*		
benomyl	150	2*	150	0.006*	0.6	2*		
carbaryl	230	2*	230	0.03*	3*	2*		
carbendazim	110	1*	110	0.03*	3	1*		
carbofuran	910	9	910	0.02*	2	9		
maneb	-	-	as ETU	2	-	-		
metam-Natrium	35*l	0.4*l	35*l	0.006*l	0.6l	0.4*l		
methomyl**	80	0.8*	80	0.001*	0.1	0.8*		
oxamyl**	1800	18	1800	0.01*	1	18		
pirimicarb	90	0.9*	90	0.02*	2	0.9*		
propoxur	10	0.1*	10	0.0001*	0.01	0.1*		
thiram	32	0.3*	32	0.008*	0.8	0.3*		
tri-allate	1900	19*	1900	0.2l	160	19*		
zineb	-	-	as ETU	130l	-	-		
<u>triazines, pyridazines & triazoles</u>		<u>ng/l</u>	<u>ng/l</u>	<u>µg/kg s.s.</u>	<u>µg/kg s.s.</u>	<u>ng/l</u>		
anilazine	85	0.9*	85	0.02*	2	0.9*		
atrazine	2900	29	2900	0.2*l	26	29		
chloridazon	73000	730	73000	3	350	730		
cyanazine**	190	2*	190	0.01*l	2	2*		
desmetryn	34000l	340l	34000l	0.08*l	370l	340l		
metamitron	10000	100	10000	1*	95	100		
simazine	140l	1*l	140l	0.009*l	0.9l	1*l		

ORGANIC SUBSTANCES (continued)	SURFACE WATER		SEDIMENT & SOIL		GROUND WATER	
	MPC (dissolved)	target value (water-total)	target value (dry matter)	MPC-sed (dry matter)	target value (dissolved)	
<u>synthetic pyrethroids</u>						
bifenthrin	1*	ng/l 0.01*	μg/kg s.s. 0.05*	μg/kg s.s. 5	ng/l 0.01*	
cypermethrin	0.09*	0.001*	0.004*	0.4	0.0009*	
deltamethrin	0.3*	0.004*	0.01*	1	0.003*	
permethrin	0.2*	0.003*	0.009*	0.9	0.002*	
<u>anilids & dinitroanilines</u>						
metazachlor	34000l	ng/l 340l	μg/kg s.s. 3	μg/kg s.s. 260	ng/l 340l	
metolachlor	200	2*	0.03*	3	2*	
propachlor**	1300	13*	0.06*	6	13*	
quintozene	2900	31*	-	-	29*	
trifluralin	37l	0.4* ^l	0.1* ^l	19l	0.4* ^l	
<u>fenylureum herbicides</u>						
diuron**	430	ng/l 4*	μg/kg s.s. 0.08* ^l	μg/kg s.s. 9	ng/l 4*	
isoproturon	320	3*	0.05*	5	3*	
linuron**	250	3*	0.09*	9	3*	
metabenzthiazuron**	1800	18*	0.7*	67	18*	
metobromuron	10000	100	1	110	100	
<u>carboximiden</u>						
captan	ng/l 28* ^l	ng/l 0.3* ^l	μg/kg s.s. 0.03l	μg/kg s.s. 3l	ng/l 0.3* ^l	
captan	110*	1*	0.01	1	1*	
<u>OTHER POLLUTANTS</u>						
not based on ecotoxicological risk thresholds						
NTA	μg/l	μg/l	μg/kg s.s.	μg/kg s.s.	μg/l	
mineral oil	-	-	-	-	0.2	
	-	-	50	1000	50	
PCBs			μg/kg s.s.	μg/kg s.s.	μg/l	
PCB-28	-	-	1	4	-	
PCB-52	-	-	1	4	-	
PCB-101	-	-	4	4	-	
PCB-118	-	-	4	4	-	
PCB-138	-	-	4	4	-	
PCB-153	-	-	4	4	-	
PCB-180	-	-	4	4	-	
sum 7-PCB	-	-	20	-	0.01*	

OTHER POLLUTANTS not based on ecotoxicological risk thresholds (continued)	SURFACE WATER			SEDIMENT & SOIL		GROUND WATER	
	MPC (dissolved)	target value (water-total)	MPC (water-total)	target value (dry matter)	MPC-sed (dry matter)	target value (dissolved)	
				<u>mg/kg s.s.</u>		<u>µg/l</u>	
cyanide (total free)	-	-	-	1	-	5	
cyanide (complex)	-	-	-	5	-	10	
thiocyanates (sum)	-	-	-	1	-	-	
phenol	-	-	-	0.05	-	0.2	
cresoles (sum)	-	-	-	0.05	-	0.2	
catechol	-	-	-	0.05	-	0.2	
resorcinol	-	-	-	0.05	-	0.2	
hydroquinon	-	-	-	0.05	-	0.2	
cyclohexanon	-	-	-	0.1	-	0.5	
phthalates (sum)	-	-	-	0.1	-	0.6	
pyridine	-	-	-	0.1	-	0.6	
tetrahydrofuran	-	-	-	0.1	-	0.5	
tetrahydrothiophene	-	-	-	0.1	-	0.5	
monochloronitrobenzene	-	-	-	0.01	-	-	
dichloronitrobenzene	-	-	-	0.01	-	-	
octane	-	-	-	0.001	-	-	
heptane	-	-	-	0.001	-	-	
hexachlorobutadiene	-	-	-	0.003	-	-	
SCREENING PARAMETERS							
EOX	-	<u>µg/l</u>	<u>µg/l</u>	<u>mg/kg s.s.</u>	<u>mg/kg s.s.</u>	-	
VOX	-	-	-	0.1*	-	-	
ETU	-	-	5	-	-	-	
cholinesterase inhibition	-	-	0.005	-	-	-	
	-	-	0.5	-	-	-	

NUTRIENTS &

EUTROPHICATION PARAMETERS

nitrate (mg N/l)
total phosphate (mg P/l)
total nitrogen (mg N/l)
(Kjeldahl N + NO₃ + NO₂)
ammonia (mg N/l)
chlorophyll-a (µg/l)
ammonium compounds (mg N/l)

SALTS

chloride (mg Cl/l)
fluoride (mg F/l)
bromide (mg Br/l)
sulphate (mg SO₄/l)
S (total sulfides)

RADIOACTIVITY

PARAMETERS

(1Bq = 27 pCi)
total α-activity (l)
rest β-activity (l)
tritium-activity (l)
radium-226
strontium-90
cesium-137
lead-210
polonium-210
cobalt-58
cobalt-60
iodium-131
other γ-radiators

SURFACE WATER

general

target value MPC
- -
0.05 (z) 0.15 (z)
1 (z) 2.2 (z)
- 0.02
- 100 (z)
- -

SEDIMENT & SOIL

target value

MPC-sed
- -
- -
- -

GROUND WATER

(dissolved)

target value
5.6 (1)
0.4 / 3.0 (1,2)
-

-
-
2 / 10 (3,4)

100 (3)
0.5 (3)
0.3 (3)
150 (3)
10 (µg/l)

SUSPENDED SOLIDS

target value

MPC
Bq/kg Bq/kg

- -
- -
- -
- -
- -
40 -
80 -
80 -
10 -
10 -
2 -
2 -

legend

*: value below detection threshold/lower determination limit or determination method lacking

**: reassessment of pesticide approval by CTB in 97/98

***: no soil type correction at organic matter content < 10 %

~: MPC4-hrs. VR4-hrs.

(-): no value established

#: value = Interventionvalue

Ind: value holds for each individual compound

! : an extra uncertainty factor of 10 is used due to limited amount of data (derivation method: EPA/1000)

n: naturally deviations are allowed

J : annual averaged value

w: winter averaged value

z : summer averaged value for stagnant waters susceptible to eutrophication

1: for the protection of oligotrophic waters lower values might be necessary

2: the value of 0.4 mg P/l holds for sandy soils, the value of 3.0 mg P/l holds for claysoil and peaty soil

3: in areas with marine influence higher values occur naturally (salt and brackish ground water)

4: the value of 2 mg N/l holds for sandy soils, the value of 10 mg N/l holds for claysoil and peaty soils

5: differentiation on soil lutum content: (F) = 175 + 13L

Notes on table 1:

Standards for metals

In deriving standards for metals, allowance was made for the fact that metals occur naturally in the environment. The standards for metals are composed of a natural background concentration and a toxicological risk limit. The natural background concentration is taken as the upper limit of the concentrations measured in relatively unpolluted areas. These national background levels are shown in the table. The MPC includes this background concentration. The target value is composed of the background concentration plus the NC. The use of a constant background level does not properly reflect the considerable natural variation, both geographical and seasonal, which occurs. Naturally occurring concentrations can vary between different locations. It is possible for the standards to be exceeded purely as a result of natural levels. However, in such situations, according to the added-risk-approach the locally occurring background concentrations can be included in the standard. Chapter 4 indicates how local differences in background concentrations can be dealt with in applying the environmental quality standards.

Zinc

A working party of the Dutch Health Council has drawn up recommendations on zinc and on a risk assessment methodology for essential elements. These recommendations have been brought in into the EU risk assessment with respect to zinc being carried out in the framework of the EU-Regulation for existing substances (Regulation 1488/94). In case the results of the EU-risk assessment, which are expected by the end of 1999, gives arguments to change the MPC and target value for zinc, the values will be adjusted.

Standard soil

The target values for soil/sediments and the MPCs for sediments are related to the levels of organic matter and/or clay in the soil. The values given in table 1 apply to a so-called 'standard soil' containing 10% organic matter and 25% clay. In assessing soils/sediments with a different composition the corrections given in Annex 2 must be applied.

MPCs for surface water: water-total and dissolved content

The MPCs for surface waters are given for both water-total and dissolved content. With respect to monitoring in practice it will usually be the total content which is measured. The MPCs for total content relate to 'standard' water with 30 mg/l suspended solids. Where the concentration of suspended solids in the water is different an adjustment will have to be applied (see Annex 1).

Pesticides

The MPCs for pesticides in the table were derived by the RIVM from published sources. They may differ from the existing approval standards for these substances. Over the next few years the Pesticides Approval Committee (CTB) will set MPCs for new pesticides and pesticides being reassessed. These MPCs will be adopted as environmental quality standards, and will be made public, for example on the Internet or in the periodical H₂O. The methodology used by the Pesticides Approval Committee to determine the MPC is similar to the procedure used within the INS project. Information on expiration data for specific pesticides is available on the internet site of the Pesticides Approval Committee (<http://www.bib.wau.nl/ctb>).

Standards based on limited scientific evidence

For some substances there are very few scientific data available. In determining toxicological risk limits for such substances an additional safety factor of 10 is applied, in accordance with international practice. The substances to which this applies are indicated in the table. Caution needs to be exercised in using these standards. If the activity responsible for causing the standard to be exceeded is of major importance in economic terms, the scientific basis for the standard will need to be improved. If no progress is made on this front, the risks involved at the site must be weighed up against the economic interests involved.

Detection thresholds/lower determination limits

There are a number of substances for which the table indicates that the standards are lower than the existing detection thresholds.

Two different sources were used for this purpose:

- detection thresholds generated by the Committee for Integrated Water Management (CIW/CUWVO). These are levels at which the presence of the substance can be detected, and are consistent with current measuring practice;
- lower determination limits from the DOMINO database. DOMINO only gives lower determination limits based on standard measurement procedures from the Netherlands Standardisation Institute. A lower determination limit is the lowest level for which the concentration of a substance can be determined with a given degree of certainty.

In order to stick as closely as possible to common measuring practice, the CIW/CUWVO detection limits were adopted. Where this was not possible DOMINO values were used.

After considering other options, it was decided that standards below the detection threshold/lower determination limit would be adopted. Developments in measuring techniques could mean that within a few years it may be possible to measure concentrations equal to the standard. Furthermore, when the standards are used to calculate emission reduction percentages the lack of measurability is irrelevant.

For substances with standards below the current detection limit it will be uncertain whether or not the standard is being exceeded if substances can not be detected (concentrations below detection limit). A positive reading, however, will mean that the standard is being exceeded.

Screening parameters

This document also includes MPCs and/or target values for several so-called screening parameters. These are not related to toxicological risk limits. Screening parameters have a mainly indicative value: where a screening parameter is exceeded, a check would be carried out to ascertain which individual substances which fall within the screening parameter are exceeding the standards. EOX includes the extractable and VOX the volatile organic halogen compounds. ETU is a conversion product of, amongst other things, maneb and zineb.

Unchanged MILBOWA standards

No change has been made to the MILBOWA standards for chlorophenols because no

assessment of the toxicological risk limits has been carried out. An evaluation was not expected to produce results which differ from the toxicological risk limits determined in the MILBOWA. The MILBOWA standards for PCBs and substances in the 'other pollutants' category were also adopted because no risk assessment was carried out for these substances.

4 Application of environmental quality standards

As indicated in the NEPP3, the relevant authorities will use the target values and MPC values as a frame of reference in:

- assessing environmental quality;
- formulating and prioritising pollution abatement policy;
- evaluating the need for legally-binding environmental quality standards;
- standard setting for product- and pesticedmanagement
- re-evaluating and formulating objectives and targets for groups of polluters;
- re-evaluating and formulating policy objectives;
- licensing activities.

In applying environmental policy, decisions will take account not only of the standards themselves, but also of technical feasibility and developments in neighbouring countries.

The standards are designed for use by various authorities, but will be particularly relevant for municipalities, water boards, provinces and central government in the fields of environmental management, planning, traffic management and industrial policy. The manner in which the standards are applied will differ between the various environmental media. This is considered further below.

Target values for soil quality

Target values have been formulated for soil and groundwater. They indicate the concentrations at which the risks can be regarded as negligible and the soil as being free of contamination. Land complying with the target values is deemed to be multifunctional, meaning that all its naturally occurring functions are safeguarded. If the target values are exceeded, risks may arise. Whether this is actually the case in a given situation will depend on the specific circumstances (soil characteristics, land-use).

The target values for soil (including groundwater) are used in policy on soil protection and the clean-up of contaminated land. The manner in which the target values are used and the consequences of exceeding the target values will depend on the context within which they are being used. In the case of soil the target values will take practical effect when they are included in specific regulations on soil protection and clean-up. It is only then that the target values will acquire force in soil policy.

In soil protection policy, the target value indicates the standard that must be maintained or achieved through soil protection measures. Target values are implemented in specific regulations intended to protect the soil, such as the Building Materials Decree and the Soil Protection (Discharges) Decree.

Until recently, target values fulfilled two functions in soil clean-up policy. They served as criteria for demarcating contaminated sites requiring clean-up and also indicated the soil quality which should, if reasonable, be aimed for in the clean-up. This is known as the 'multifunctional, unless ...' approach. In September 1997 the Government statement on the updated policy on contaminated land was formally adopted by the Second Chamber (Second Chamber). In this, the government indicated that for 'old' cases of contaminated land (i.e.

cases which pre-date the 1987 Soil Protection Act) the 'multifunctional, unless ...' approach was to be abandoned, to be replaced by a function-specific clean-up for non-mobile contamination and a cost-effective approach to clean-up in the case of mobile contamination. This is leading to a change in the way target values are being used in soil clean-up policy. A clean-up which achieves the target values means that the contaminated land has been restored to a multifunctional status. Since multifunctionality is no longer the primary end-objective, there will in practice be many cases where remediation carried out to a standard above the target value is accepted.

Target values for ground water

As is indicated in Chapter 3 measured concentrations of substances in shallow groundwater bodies can not directly be compared with the presented environmental quality standards for groundwater, as they hold for deep groundwater bodies (>10 meter). In a new Circular containing target and intervention values (to be published in 1999) the use of the target values for shallow groundwater bodies will be indicated.

Aggregated target values for soil

Individual target values are given in this document for a number of substances while intervention values are specified for groups of substances (PAH, DDT/DDE/DDD, drins, HCH compounds, chlorophenols, chlorobenzenes and organotin compounds): see 1994 and 1997 Circulars containing intervention values for soil. In order to provide for consistency between the intervention values and the target values, individual target values will not be set for the substances concerned in soil; instead, target values will be set for each group. In setting these values, account will also be taken of concentrations in relatively unpolluted areas (TNO/IWACO 1997).

MPCs and target values for the quality of water and sediments

Within the aquatic medium standards have been formulated for surface waters (total and dissolved component of pollutant) and sediments. The standards for total content of a particular pollutant in surface water relate to standard water with 30 mg/l suspended solids. Analysis results should therefore be corrected for the actual concentration of suspended solids.

The measured concentrations of organic micropollutants in sediment need to be standardised to allow for the organic matter content, and the concentrations of metals in sediments need to be standardised to allow for the organic matter and clay content in the samples concerned. The standardised concentrations can then be tested against the MPC and target value for 'standard' soil. The formulae for soil and for sediments are given in Annex 2. The standardisation can be carried out by a computer model maintained by RIZA (Institute for Inland Water Management and Wastewater Treatment), the software for which (BOOS, 1997) is available free-of-charge to all water boards. Jonkers et al. (1992) give the current formulae for standardising concentrations of organic micropollutants and metals in brackish and marine sediments.

The partition coefficients used in this model are presented in Annex 1. The formulae presented allow the standardisation to be carried out without using the RIZA model.

The Committee for Integrated Water Management (CIW/CUWVO) has made recommendations as to which substances should be monitored. They have also drawn up guidelines for evaluating the results. A CUWVO-report (1990)³ contains general guidelines on sampling methods and the number of samples to be taken per aquatic system.

Sumpparameter-based assessment

It is possible to evaluate groups of substances which act in similar ways, such as organophosphate pesticides and carbamates or PAHs, by carrying out an assessment using an aggregated MPC level ('sumparameter'), in addition to a substance-specific assessment. This is done by adding together the ratios of 'measured concentration/MPC' for the different substances. This sumparameter has only an indicative value, but can help to further prioritise environmental management activities. The CIW, RIZA and the National Institute for Coastal and Marine Management will examine the possibility of using such aggregates for the aquatic medium (i.e. including sediments) in greater detail in the near future.

Bioassays

Bioassays are laboratory tests in which organisms are directly exposed to samples taken from, for example, surface waters, effluents or sediments. Bioassays give indications of the overall effects of combinations of known, measured substances and unknown, unmeasured substances. Bioassays are increasingly used to supplement tests of samples against substance-specific standards, in assessing the quality of surface water, waste water, dredging spoil and sediments. Criteria for assessing the results of bioassays for water and sediments, in the form of MPCs and target values, are proposed in the Fourth Policy Document on Water Management.

For the moment the main focus of bioassays is on their use as a warning and monitoring instrument. The assessment criteria (MPC, target value) do not entail an obligation to take action, but do invite it. The Committee for Integrated Water Management has been asked to develop recommendations for the use of bioassays in monitoring programmes for the aquatic environment (including sediments).

Air quality standards

New air quality target values have only been developed for a limited number of substances within the INS project. These are substances for which the only known emitters are companies. It is therefore not appropriate to test these substances against the standards in urban areas characterised by heavy traffic. For other substances for which statutory air quality limit values have been formulated in the past, such an evaluation is of course appropriate. In this connection, readers are referred to the relevant decrees on air quality.

The new INS air quality standards will in practice only be used for assessing process emissions to the atmosphere in the licensing procedure. The Dutch Emission Guidelines for air provide guidance to licensing authorities. These Guidelines are based on the state-of-the-art technology. Licensing authorities should evaluate the environmental impact of the residual emissions after the application of the Emission Guidelines. If these residual emissions result

³ The CIW is currently rewriting this report, which will be published in 1998 as the '*Handboek monitoring*' (Monitoring Manual).

in standards being exceeded, the competent authority can impose more stringent requirements than specified in the Emission Guidelines, limit the level of activity or refuse a licence. The grounds for such a decision must be given.

In practice, ground-level concentrations due to industrial emissions will be estimated using atmospheric dispersion models. In general the concentrations of the relevant substances will be dominated by the emissions from the establishment concerned, and background concentrations will play a negligible role. A model based on the National Air Pollution Dispersion Model is used for the calculations. There are various computer versions of this model (e.g. PluimPlus). The National Model was recently revised at the request of the Ministry of Housing, Spatial Planning & the Environment and the Association of Provincial Authorities. Computer versions of the revised model are expected to be available shortly.

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Annex 1

Partition coefficients for suspended solids in surface waters

This Annex contains a table with water/suspended solids partition coefficients which permit surface water standards for water-total to be corrected for the suspended solids content and the standards for water (total) to be converted to dissolved components and vice versa. The conversion method is described below.

Conversion from dissolved components to water-total

The standards for water-total assume a suspended solids content of 30 mg/l comprising a standard 20% organic matter and 40% clay. A soil type correction, applied to the figures for standard suspended solids, is used for suspended solids of different characteristics, as indicated in Annex 2.

Metals

The standards for metals are equal to the sum of the toxicological risk limit and the national background concentration. The MPC or the target value can be adjusted appropriately to reflect local background concentrations.

In order to convert from water-dissolved to water-total and vice versa, partition coefficients are used (see table 1). These apply to the risk threshold component of the MPC or target value, i.e. excluding the background concentration. After the conversion from water-dissolved to water-total (or vice versa), the appropriate background concentration should be added back in again.

The conversion formula is as follows:

$$\text{MPC}_{\text{total}} = (\text{MPC}_{\text{dissolved}} - \text{BC}_{\text{dissolved}}) + \{(\text{MPC}_{\text{dissolved}} - \text{BC}_{\text{dissolved}}) * K_p * 0.001 * 0.03\} + \text{BC}_{\text{total}}$$
$$\text{Target value} = (0.01 * \{\text{MPC}_{\text{total}} - \text{BC}_{\text{total}}\}) + \text{BC}_{\text{total}}$$

where:

BC = background concentration.

K_p = partition coefficient water/suspended solids (see table 1).

0.03 = suspended solids content of 30 mg/l; if the actual suspended solids content differs from this value, the actual value should be inserted here.

These partition coefficients cannot be used to convert from the value for water-total to the value for sediments or vice versa.

Organic compounds

The partition coefficients in table 1 can be used to convert the standards for organic compounds for water-dissolved to those for water-total and also to those for sediments. The conversion is based entirely on differences in the percentage of organic matter. The conversion formulae are as follows:

$$\text{MPC}_{\text{sediment}} = \text{MPC}_{\text{water-dissolved}} * K_p * 0.5$$
$$\text{MPC}_{\text{total}} = \text{MPC}_{\text{dissolved}} + (\text{MPC}_{\text{dissolved}} * K_p * 0.001 * 0.03)$$

where:

K_p = partition coefficient water/suspended solids (see table 1).

The target values are equal to $1/100 * \text{MPC}$.

ENVIRONMENTAL QUALITY STANDARDS FOR SOIL, WATER AND AIR
Annex 1: partition-coefficients for suspended solids in surface waters

metals: Kp in l/kg suspended solids, for standard suspended solids containing 20 % organic carbon and 40 % lutum

other substances: values as log Kp (l/kg) voor standard suspended solids

Partition coefficients for standard sediment (10% organic carbon, 25% lutum): values for metals are 0.67 times the values for suspended solids and for organic substances 0.5 times the values for suspended solids

METALS		METALS		ORGANIC SUBSTANCES	
	Kp l/kg susp.solids	(continued)	Kp l/kg susp.solids	(continued)	log Kp l/kg susp.solids
cadmium	130.000	antimony	3.700	<u>organotin compounds</u>	
mercury (Inorganic)	170.000	barium	1.350	tetrabutyltins (Ind)	1.99
methyl-mercury	170.000	beryllium	850	tributyltins (Ind)	3.17
copper	50000**	cobalt	3.900*	triphenyltins (Ind)	3.41
nickel	8.000	molybdenum	1.120	<u>acids</u>	
lead	640000**	selenium	590	benzoxone	0.59
zinc	110.000	thallium	1.500	2,4-D	0.73
chromium	290000**	tin	371.500*	dichlorprop	2.2
arsenic	10.000	vanadium	5500**	dlnoseb	1.34
				dlnoterb	2.81
				DNOC	1.41
				MCPA	0.8
				mecoprop	-0.009
				2,4,5-T	1.06
ORGANIC SUBSTANCES		ORGANIC SUBSTANCES		ORGANIC SUBSTANCES	
	log Kp l/kg susp.solids	(continued)	log Kp l/kg susp.solids		
<u>PAHs</u>		<u>chlorophenols</u>		<u>carbamates & dithio-carbamates</u>	
naphthalene	2.37	monochlorophenols (In	1.2	aldicarb	0.29
anthracene	3.52	dichlorophenols (Ind)	1.6	benomyl	0.91
phenanthrene	3.53	trichlorophenols (Ind)	1.9	carbaryl	1.33
fluoranthene	4.23	tetrachlorophenols (Ind)	2.25	carbendazim	1.68
benzo(a)anthracene	4.86	pentachlorophenol	2.23	carbofuran	0.6
chrysene	4.8			maneb	-
benzo(k)fluoranthene	5.07	<u>chlorinated organics</u>		metam-Natrium	1.5
benzo(a)pyrene	5.04	aldrin	4.11	methomyl	0.43
benzo(ghi)perylene	5.7	dieldrin	4.87	oxamyl	0.12
indeno(123-cd)pyrene	5.47	endrin	3.29	pirimicarb	1.69
		DDT	4.63	propoxur	0.42
<u>volatile halogenated hydrocarbons</u>		DDD	3.91	thiram	1.69
monochlorobenzene	1.41	DDE	3.82	tri-allate	2.19
dichlorobenzenes (Ind)	1.71	α-endosulphan	2.11	zinab	-
trichlorobenzenes (Ind)	2.38	α-HCH	2.25		
tetrachlorobenz. (Ind)	2.85	β-HCH	3.36	<u>triazins, pyridazins & triazoles</u>	
pentachlorobenzene	2.9	γ-HCH (lindane)	2.7	anilazine	1.71
hexachlorobenzene	3.04	heptachlor	3.45	atrazine	1.27
		heptachlorepoxyde	1.94	chloridazon	0.98
		chlordan	3.6	cyanazine	1.33
				desmetryn	1.34
benzene	0.87	<u>organophosphorus compounds</u>		metamitron	1.27
acrylonitril	-0.68	azinphos-ethyl	1.94	simazine	1.11
3-chloropropene	0.52	azinphos-methyl	2.17		
dichloroethanes (Ind)	0.33	chlorfenvinphos	2.19	<u>synthetic pyrethroids</u>	
1,1-dichloroethene	0.93	chlorpyrifos	2.88	bifenthrin	3.94
1,2-dichloroethene	0.83	coumaphos	2.34	cypermethrin	3.94
dichloromethane	0.63	demeton	-	deltamethrin	3.94
1,2-dichloropropane	0.68	diazinon	1.73	permethrin	3.94
1,3-dichloropropane	0.68	dichlorvos	0.9		
1,3-dichloropropene	0.76	dimethoate	0.83	<u>anilids & dinitroanilines</u>	
2,3-dichloropropene	1.04	disulfoton	2.18	metazachlor	1.18
ethene	0.15	ethopros	0.98	metolachlor	1.4
ethylbenzene	1.3		2.2	propachlor	0.98
ethylenoxide	-1.32	fenthion	2.35	quintozene	3.36
hexachloroethane	2.68	foxim	2.3	trifluralin	3
monochlorotoluenes (In	2.33	heptenofos	1.47		
pentachloroethane	2.7	malathion	2.14	<u>fenylureum-herbicides</u>	
styrene	2.02	mevinfos	1.87	diuron	1.62
1,1,2,2-tetrachlorethane	0.99	oxydemeton-methyl	0.18	isoproturon	1.52
tetrachlorethane	1.45	parathion(-ethyl)	2.12	linuron	1.85
tetrachloromethane	1.9	parathion-methyl	2.24	metabenzthiazuron	1.87
toluene	1.15	pyrazofos	2.09	metobromuron	1.34
1,1,1-trichlorethane	0.89	tolclofos-methyl	2.62		
1,1,2-trichlorethane	1.06	triazophos	1.62	<u>carboximides</u>	
trichlorethane	1.11	trichlorfon	0.65	captan	2.38
trichloromethane	0.88			captan	1.37
vinylchloride	0.59				
xylene (Ind)	1.87				

legend

*: Kp-sediment = Kp-suspended solids

** : Kp-sediment differs more than factor 1.5 from Kp-suspended solids

(Ind): values for individual compounds identical. Kp is calculated from MTR-sediment and MTR-water-dissolved and holds for each individual substance

(-): no value established

Annex 2

Soil type correction

The standards for soil/sediments in table 1 are given for a 'standard' soil (25% clay and 10% organic matter). A correction must be applied for soil/sediments with other clay and organic matter contents.

Metals

The standards for metals in soil/sediment depend on the clay content and/or the organic matter content. In assessing soil quality, the standards for a standard soil are converted to standards applying to the actual soil and are then compared with the measured values for the soil/sediment. Alternatively, the measured values can be converted to values applying for a standard soil and then compared with the standard applying to a standard soil. These two methods give the same results. The conversion is based on the measured organic matter content (loss of weight on ignition as a percentage of total dry weight) and clay content (weight of mineral components with a diameter less than 2 mm as a percentage of the total dry weight of the soil).

The conversion is carried out using the soil type correction formula:

$$S_a = S_{st} \times \frac{A + B \times \% \text{clay} + C \times \% \text{org. matter}}{A + B \times 25 + C \times 10} \quad (1)$$

where:

S_a = standard (MPC or target value) applying to soil being assessed (mg/kg)

S_{st} = standard (MPC or target value) for the standard soil (mg/kg)

$\% \text{clay}$ = measured percentage clay in the soil

$\% \text{org. matter}$ = measured percentage organic matter in the soil

A, B, C = constants for the substance (table 2)

For non-metal inorganic compounds the standards are not related to the soil characteristics; the same standards apply to all soils.

Organic compounds

The standards for organic compounds are related to the organic matter content of the soil. In assessing soil quality the values for a standard soil are divided by 10 and multiplied by the measured organic matter content. The resulting values can be compared with the measured concentrations of organic compounds. As for metals it is possible to perform the conversion the other way round, i.e. to convert the measured concentrations in the soil to values applying to a standard soil, and to compare these with the standards for a standard soil.

The conversion formula is as follows:

$$S_a = S_{st} \times \frac{\% \text{org. matter}}{10} \quad (1)$$

where:

S_a = standard (MPC or target value) applying to actual soil being assessed (mg/kg)

$S_{st} =$ standard (MPC or target value) for standard soil (mg/kg)
 $\%org. Matter =$ measured percentage of organic matter in the soil. For all standards for organic micropollutants other than PAH, if the measured organic matter content is more than 30% or less than 2%, values of 30% and 2% respectively should be used in the formula. In the case of PAH, if the measured organic matter content is more than 30% or less than 10%, values of 30% and 10% respectively should be used.

Standards for groundwater

The standards for both inorganic and organic compounds in groundwater are independent of soil type.

Table 2 Substance-dependent constants for metals

substance	A	B	C
antimony ¹	1	0	0
arsenic	15	0,4	0,4
barium	30	5	0
beryllium	0,3	0,033	0
cadmium	0,4	0,007	0,021
chromium	50	2	0
cobalt	2	0,28	0
copper	15	0,6	0,6
mercury	0,2	0,0034	0,0017
lead	50	1	1
molybdenum ¹	1	0	0
nickel	10	1	0
selenium ¹	1	0	0
thallium ¹	1	0	0
vanadium	12	1,2	0
zinc	50	3	1,5

¹ A soil type correction is not applied for antimony, molybdenum, selenium and thallium.

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Readers guide

In Part II of the present file, entitled "Risk limits", the procedure described in part I (entitled "Procedure"), is applied on approximately 100 substances. This procedure results in harmonized quality objectives for the environmental compartments surface water, soil, sediment and air for each individual substance. Only for the different chlorophenols (mono-, di-, tri- and tetrachlorophenols) documents are prepared for each isomer group.

The structure of each of the following documents on substances, in which the derivation of the harmonized quality objectives (i.e. MPC and NC values) is explained, is based on the above mentioned procedure.

Each document starts with an introduction (§ 1) in which general information on the substance (e.g. application) is given. If relevant, remarks are made on the natural occurrence of the substance in the environment and its bioaccumulation potential.

In the second paragraph (§ 2) the data used for the derivation of the harmonized quality objectives are described. These data include data on identification and physico-chemical properties (§ 2.1), ecotoxicity data (§ 2.2) and, if available, (human) toxicity data (§ 2.3). In § 2.2 the ecotoxicity data are described shortly. The actual data are presented in Part III. Furthermore, in the description of the available ecotoxicity data (§ 2.2), a subdivision in environmental compartments is made. In case a substance has a bioaccumulation potential, data used for the derivation of an MPC for secondary poisoning are also evaluated in this subparagraph.

The (human) toxicity data (§ 2.3) are discussed according to (sub) chronic toxicity and to three categories of toxicological endpoints, i.e. mutagenicity and carcinogenicity, teratogenicity and reproduction, and other effects. The available human studies are given as a separate item. If available, only the actual toxicity data of organisms exposed to air are presented in Part III.

In the third paragraph (§ 3) the derivation of the quality objectives is explained for each compartment, i.e. surface water (§ 3.1), soil (§ 3.2), sediment (§ 3.3) and air (§ 3.4). In addition, the motivation on the applied extrapolation method is given. In case the described substance has a bioaccumulation potential, an MPC based on direct as well as indirect effects is given, resulting in a final MPC per compartment.

In this paragraph an overview is also given of MPCs and NCs (§ 3.5).

In the fourth paragraph (§ 4), the applied harmonization procedure is explained.

The units used to express tested concentrations, MPCs or NCs are the following:

- for surface water or groundwater the concentrations are given in $\mu\text{g/l}$ or mg/l dissolved material;
- for sediment and soil the concentrations are expressed in mg/kg dry weight. All the concentrations are determined for a standard sediment or soil, e.g. a sediment or soil containing 25% lutum (clay) and 10% organic matter;
- for air the concentrations are given in $\mu\text{g/m}^3$ or mg/m^3 .

Following all documents on the substances, an overall list of references is given.

The evaluated substances are classified in the following groups:

- A. Monocyclic aromatic hydrocarbons;
- B. Polycyclic aromatic hydrocarbons;
- C. Aliphatic hydrocarbons;
- D. Pesticides.

Within the different groups, the substances are ordered alphabetically.

Next, a summarizing table is given with all derived MPCs and NCs for the compartments surface water, soil, sediment and air. The substances in this table are ordered alphabetically.

Summarizing table

Table 1: Overview of MPCs and NCs

Substance	MPC surface water $\mu\text{g/l}$ (dissolved material)	NC surface water $\mu\text{g/l}$ (dissolved material)	MPC soil mg/kg (dry weight)	NC soil mg/kg (dry weight)	MPC sediment mg/kg (dry weight)	NC sediment mg/kg (dry weight)	MPC air $\mu\text{g/m}^3$	NC air $\mu\text{g/m}^3$
Acrylonitrile	7.6	0.076	$6.8 \cdot 10^{-4}$	$6.8 \cdot 10^{-6}$	$6.8 \cdot 10^{-4}$	$6.8 \cdot 10^{-8}$	10	-
Aldrin	0.018	$1.8 \cdot 10^{-4}$	0.050	$5.0 \cdot 10^{-4}$	0.12	0.0012	-	-
Anthracene	0.07	0.0007	0.12	0.0012	0.12	0.0012	-	-
Benzene	240	2.4	0.95	0.0095	0.95	0.0095	12 ¹	0.12 ²
Benzo(a)anthracene	0.01	0.0001	0.25	0.0025	0.36	0.0036	-	-
Benzo(a)pyrene	0.05	0.0005	0.26	0.0026	2.7	0.027	1.0	0.01
Benzo(k)fluoranthene	0.04	0.0004	2.4	0.024	2.4	0.024	-	-
Carbofuran	0.015	$1.5 \cdot 10^{-4}$	0.0047	$4.7 \cdot 10^{-5}$	$3.2 \cdot 10^{-5}$	$3.2 \cdot 10^{-7}$	-	-
Chlordane	0.0015	$1.5 \cdot 10^{-5}$	0.0043	$4.3 \cdot 10^{-5}$	0.0080	$8.0 \cdot 10^{-5}$	-	-
2-Chloro-1,3-butadiene	-	-	-	-	-	-	1.0	0.010
3-Chloropropene	3.4	0.034	0.0048	$4.8 \cdot 10^{-5}$	0.0048	$4.8 \cdot 10^{-5}$	7.4	0.074
Chlorpyrifos	0.0028	$2.8 \cdot 10^{-5}$	0.0011	$1.1 \cdot 10^{-5}$	0.0011	$1.1 \cdot 10^{-5}$	-	-
DDD	$4.4 \cdot 10^{-4}$	$4.4 \cdot 10^{-6}$	0.010	$1.0 \cdot 10^{-4}$	0.0018	$1.8 \cdot 10^{-5}$	-	-
DDE	$4.4 \cdot 10^{-4}$	$4.4 \cdot 10^{-6}$	0.010	$1.0 \cdot 10^{-4}$	0.0015	$1.5 \cdot 10^{-5}$	-	-
DDT	$4.4 \cdot 10^{-4}$	$4.4 \cdot 10^{-6}$	0.010	$1.0 \cdot 10^{-4}$	0.0094	$9.4 \cdot 10^{-5}$	-	-
1,2-Dichlorobenzene	250	2.5	5.5	0.055	5.5	0.055	60	0.60
1,3-Dichlorobenzene	250	2.5	0.40	0.0040	5.5	0.055	-	-
1,4-Dichlorobenzene	250	2.5	0.40	0.0040	5.5	0.055	670	6.7
1,1-Dichloroethane	700	7.0	1.5	0.015	1.5	0.015	370	3.7
1,2-Dichloroethane	700	7.0	1.5	0.015	1.5	0.015	100	-
1,1-Dichloroethene	3,400	34	12	0.12	12	0.12	200	2.0

Substance	MPC surface water $\mu\text{g/l}$ (dissolved material)	NC surface water $\mu\text{g/l}$ (dissolved material)	MPC soil mg/kg (dry weight)	NC soil mg/kg (dry weight)	MPC sediment mg/kg (dry weight)	NC sediment mg/kg (dry weight)	MPC air $\mu\text{g/m}^3$	NC air $\mu\text{g/m}^3$
1,2-Dichloroethene	6,100	61	22	0.22	22	0.22	36	0.36
Dichloromethane	20,000	200	36	0.36	36	0.36	25,000 ³	20 ⁴
Dichlorophenols	15	0.15	0.20	0.0020	0.33	3.3*10 ⁻³	-	-
1,2-Dichloropropane	76	0.76	4.2	0.042	0.18	1.8*10 ⁻³	12	0.12
1,3-Dichloropropane	76	0.76	0.18	1.8*10 ⁻³	0.18	1.8*10 ⁻³	6,000	60
1,3-Dichloropropene	8.0	0.080	0.023	2.3*10 ⁻⁴	0.023	2.3*10 ⁻⁴	40	0.40
2,3-Dichloropropene	8.0	0.080	0.044	4.4*10 ⁻⁴	0.044	4.4*10 ⁻⁴	380	3.8
Dieldrin	0.018	1.8*10 ⁻⁴	0.050	5.0*10 ⁻⁴	0.67	0.0067	-	-
Endosulfan	4.0*10 ⁻⁴	4.0*10 ⁻⁶	0.050	5.0*10 ⁻⁴	2.6*10 ⁻⁵	2.6*10 ⁻⁷	-	-
Endrin	0.0030	3.0*10 ⁻⁵	0.0029	2.9*10 ⁻⁵	0.0029	2.9*10 ⁻⁵	-	-
Ethylbenzene	370	3.7	3.1	0.031	3.1	0.031	39	0.39
Ethylene	8,500	85	5.8	0.058	5.8	0.058	-	2
Ethylene oxide	84	0.84	0.0021	2.1*10 ⁻⁵	0.0021	2.1*10 ⁻⁵	3.0	-
Fenthion	0.0031	3.1*10 ⁻⁵	3.5*10 ⁻⁴	3.5*10 ⁻⁶	3.5*10 ⁻⁴	3.5*10 ⁻⁶	-	-
Fluoranthene	0.30	0.0030	2.6	0.026	2.6	0.026	-	-
α -HCH	2.5	0.025	0.22	2.2*10 ⁻³	0.22	2.2*10 ⁻³	-	-
β -HCH	0.080	8.0*10 ⁻⁴	0.092	9.2*10 ⁻⁴	0.092	9.2*10 ⁻⁴	-	-
Heptachlor	4.6*10 ⁻⁴	4.6*10 ⁻⁶	7.0*10 ⁻⁴	7.0*10 ⁻⁶	6.5*10 ⁻⁴	6.5*10 ⁻⁶	-	-
Heptachlor epoxide	4.6*10 ⁻⁴	4.6*10 ⁻⁶	7.0*10 ⁻⁴	7.0*10 ⁻⁶	2.0*10 ⁻⁶	2.0*10 ⁻⁷	-	-
Hexachlorobenzene	0.0021	2.1*10 ⁻⁵	0.028	2.8*10 ⁻⁴	0.0012	1.2*10 ⁻⁵	2.3	0.023
Hexachloroethane	83	0.83	17	0.17	17	0.17	27	0.27
Lindane	0.77	7.7*10 ⁻³	0.0050	5.0*10 ⁻⁵	0.19	0.0019	-	-
Monochlorobenzene	690	6.9	7.6	0.076	7.6	0.076	42	0.42
Monochlorophenols	25	0.25	0.20	0.002	0.22	2.2*10 ⁻³	-	-
2-Monochlorotoluene	310	3.1	33	0.33	33	0.33	780	7.8

Substance	MPC surface water $\mu\text{g/l}$ (dissolved material)	NC surface water $\mu\text{g/l}$ (dissolved material)	MPC soil mg/kg (dry weight)	NC soil mg/kg (dry weight)	MPC sediment mg/kg (dry weight)	NC sediment mg/kg (dry weight)	MPC air $\mu\text{g/m}^3$	NC air $\mu\text{g/m}^3$
3-Monochlorotoluene	310	3.1	33	0.33	33	0.33	-	-
4-Monochlorotoluene	310	3.1	33	0.33	33	0.33	-	-
Naphthalene	1.2	0.012	0.14	0.0014	0.14	0.0014	-	-
Pentachlorobenzene	0.030	3.0×10^{-4}	0.12	1.2×10^{-3}	0.012	1.2×10^{-4}	-	-
Pentachloroethane	230	2.3	49	0.49	49	0.49	-	-
Pentachlorophenol	2.0	0.020	0.20	0.0020	0.17	1.7×10^{-3}	-	-
Phenanthrene	0.30	0.0030	0.51	0.0051	0.51	0.0051	-	-
Quintozene	0.29	2.9×10^{-3}	0.33	3.3×10^{-3}	0.33	3.3×10^{-3}	-	-
Styrene	570	5.7	25	0.25	25	0.25	800	-
TBTO	0.003	3.0×10^{-5}	0.003	3.0×10^{-5}	0.003	3.0×10^{-5}	-	-
1,2,3,4-Tetrachlorobenzene	24	0.24	0.072	7.2×10^{-4}	7.2	0.072	1.6	0.016
1,2,3,5-Tetrachlorobenzene	24	0.24	0.072	7.2×10^{-4}	7.2	0.072	1.6	0.016
1,2,4,5-Tetrachlorobenzene	24	0.24	0.072	7.2×10^{-4}	7.2	0.072	1.6	0.016
1,1,2,2-Tetrachloroethane	3,300	33	14	0.14	14	0.14	0.20	0.0020
Tetrachloroethene	330	3.3	0.16	0.0016	4.0	0.040	250	2.5
Tetrachloromethane	1,100	11	37	0.37	37	0.37	60	-
Tetrachlorophenols	1.0	0.010	0.3	0.003	0.086	8.6×10^{-4}	-	-
Thiram	0.032	3.2×10^{-4}	0.038	3.8×10^{-4}	7.9×10^{-4}	7.9×10^{-6}	-	-
Toluene	730	7.3	1.4	0.014	4.2	0.042	3000	30
1,2,3-Trichlorobenzene	67	0.67	0.24	0.0024	6.7	0.067	4.0	0.040
1,2,4-Trichlorobenzene	67	0.67	0.24	0.0024	6.7	0.067	4.0	0.040
1,3,5-Trichlorobenzene	67	0.67	0.24	2.4×10^{-3}	6.7	0.067	4.0	0.040
1,1,1-Trichloroethane	2,100	21	6.9	0.069	6.9	0.069	4,800	48
1,1,2-Trichloroethane	7,900	79	39	0.39	39	0.39	18	0.18
Trichloroethane	2,400	24	13	0.13	13	0.13	5,000	50
Trichloromethane	590	5.9	1.9	0.019	1.9	0.019	100	1.0

Substance	MPC surface water $\mu\text{g/l}$ (dissolved material)	NC surface water $\mu\text{g/l}$ (dissolved material)	MPC soil mg/kg (dry weight)	NC soil mg/kg (dry weight)	MPC sediment mg/kg (dry weight)	NC sediment mg/kg (dry weight)	MPC air $\mu\text{g/m}^3$	NC air $\mu\text{g/m}^3$
Trichlorophenols	2.5	0.025	0.04	0.0004	0.10	1.0×10^{-4}	-	-
Vinylchloride	820	8.2	1.4	0.014	1.4	0.014	100	-
2-Xylene	380	3.8	14	0.14	14	0.14	340	3.4
3-Xylene	380	3.8	14	0.14	14	0.14	1,000	10
4-Xylene	380	3.8	14	0.14	14	0.14	1,000	10

- 1 the official limit value for benzene is $10 \mu\text{g/m}^3$
- 2 the official target value for benzene is $1 \mu\text{g/m}^3$
- 3 value applicable for 4 hours of exposure
- 4 yearly average value

Legend:

- the MPCs and NCs in surface water is expressed in $\mu\text{g/l}$ dissolved material;
- the MPCs and NCs in soil and sediment are expressed in mg/kg dry weight. All the concentrations are determined for a standard soil, e.g. a soil containing 25% clay and 10% organic matter;
- the MPCs and NCs in air are expressed in $\mu\text{g/m}^3$.

Table 2: Overview of critical concentrations rainwater and air

Substance	Critical concentration rainwater ($\mu\text{g/l}$)	Critical concentrations air ($\mu\text{g/m}^3$)
Aldrin	10	21
Anthracene	6.5	8.6
Benzo(a)anthracene	5	0.2
Benzo(k)fluoranthene	47	0.2
Carbofuran	2	0.0005
Chlordane	0.02	0.05
Chlorpyrifos	0.5	0.07
Dieldrin	0.4	0.13
Endosulfan	46	12
Endrin	0.02	0.0002
Fenthion	0.06	0.0005
Fluoranthene	54	13
α -HCH	34	12
β -HCH	15	0.77
Heptachlor	0.02	0.2
Heptachlor epoxide	0.02	0.02
Hexachlorobenzene	0.2	1.2
Lindane	0.25	0.01
Naphthalene	7.8	140
Pentachlorobenzene	9	1.5
Pentachlorofenol	56	1.1
Phenanthrene	28	33
p,p'-DDD	0.07	0.004
p,p'-DDE	0.07	0.02
p,p'-DDT	0.07	0.001
Quintozone	2.6	740
Thiram	51	1.4

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APPENDIX A

MONOCYCLIC AROMATIC HYDROCARBONS

- BENZENE
- 1,2-DICHLOROBENZENE
- 1,3-DICHLOROBENZENE
- 1,4-DICHLOROBENZENE
- DICHLOROPHENOLS
- ETHYLBENZENE
- HEXACHLOROBENZENE
- MONOCHLOROBENZENE
- 2-MONOCHLOROTOLUENE
- 3-MONOCHLOROTOLUENE
- 4-MONOCHLOROTOLUENE
- PENTACHLOROBENZENE
- PENTACHLOROPHENOL
- STYRENE
- 1,2,3,4-TETRACHLOROBENZENE
- 1,2,3,5-TETRACHLOROBENZENE
- 1,2,4,5-TETRACHLOROBENZENE
- TETRACHLOROPHENOLS
- TOLUENE

- 1,2,3-TRICHLOROBENZENE
- 1,2,4-TRICHLOROBENZENE
- 1,3,5-TRICHLOROBENZENE
- TRICHLOROPHENOLS
- 1,1,2-TRICHLOROETHANE
- 2-XYLENE
- 3-XYLENE
- 4-XYLENE

BENZENE

1. Introduction

Benzene is a volatile liquid. It is used in the Netherlands in fuel and in the production of ethylbenzene, styrene, phenol and cyclohexane. Its use as a solvent has been reduced greatly in the last few years, especially as a result of its replacement by toluene. However, the compound still occurs in small quantities in various solvents on a hydrocarbon basis (Slooff, 1988).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 71-43-2

Molecular formula : C_6H_6

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for benzene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
78.11	0.142	2.19	4.0	4.0	1.28	Yes	12.7

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-5}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater and marine organisms. For freshwater, acute data are available on algae, hydrozoa, hirudinea, oligochaeta, crustaceans, insects, molluscs, fish and amphibia. Chronic data are available on bacteria, algae, protozoa and nematoda. For marine organisms, acute data are available on algae, rotatoria, crustaceans, molluscs and fish. Chronic data are available on algae and crustaceans (part II; appendix A). The lowest NOEC is 180 $\mu g/l$ for crustaceans (Van de Plassche et al., 1993).

Because benzene is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , acute as well as chronic data for mammals (rats and mice) are available (part II; appendix A). An acute study with mice resulted in an LC_{50} of 5,000 mg/m^3 . The lowest NOAEL is 4.7 mg/m^3 for reproduction in rats, calculated as $LOAEL/10$ (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are based mainly on the integrated criteria document on benzene (Slooff, 1988).

(Sub)chronic toxicity

(Sub)chronic studies have been performed with rats and mice. The principal toxic effect after exposure is in the blood and the blood-forming tissues. In a 72-week study with mice, significant bone marrow hypoplasia (consisting of a reduction in all cell types) has been observed after exposure of 6 hours per day and 5 days per week. A concentration of 150 mg/m^3 can be regarded

as a NOAEL (Snyder et al., 1978^b).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. In in-vitro tests positive results were observed in assays with *Bacillus subtilis*, *Escherichia coli*, human lymphocytes and ovary cells and lung cells of the chinese hamster. Negative results were found in the Ames test (De Flora et al., 1984; Seixas et al., 1982; Rozenkranz and Leifer, 1980; Styles and Richardson, 1984; Morimoto et al., 1983). Benzene vapour induced chromosome abnormalities in rats after 6 hours exposure to 325 and 3,250 mg/m³, whilst no significant effects were observed at 32.5 mg/m³ (Styles and Richardson, 1984). Toft et al. (1982) demonstrated increased frequencies of micronuclei at concentrations > 63 mg/m³ subsequent to exposure of male mice by inhalation (4 to 10 days) to 3 to 600 mg/m³.

The results of several carcinogenicity studies are available (Slooff, 1988). These data show that benzene is carcinogenic in rats and mice by inhalation. A dose-related increase in the incidence of zymbal gland carcinomas was noted (Maltoni et al., 1982^a and 1982^b) after exposure to 640 mg/m³ for 4 hours per day, 5 days per week for 7 weeks and subsequently 7 hours per day, 5 days per week for 12 weeks. A slight increase in the incidence of leukaemia (Snyder et al., 1978^a), hepatocarcinomas and lymphoreticular neoplasia (Sandmeyer, 1982) was also observed.

Teratogenicity and reproduction

Teratogenicity and reproduction studies have also been performed on rats and mice (Slooff, 1988). No teratogenic effects were noted at tested concentrations lower than those which produce maternal toxicity (Hudak and Ungvary, 1978). In an inhalation study in which rats, guinea pigs and rabbits were exposed to 256 to 281 mg/m³ for 7 hours per day for 30 to 40 weeks, increased testicular weight and degeneration of seminiferous tubules were observed (Wolf et al., 1956).

Human studies

Many human studies are available about the effects of benzene on humans. Acute exposure to 65,000 mg/m³ may cause death. Adverse effects (anaemia, leucopenia) have been observed in workers exposed to 130 to 260 mg/m³ (Hardy and Elkins, 1948). Enzyme changes within the leucocytes have been observed after exposure to 32.5 to 81 mg/m³ during at least a 3-year period. Rinsky et al. (1981) reported on a retrospective cohort analysis among 748 workers exposed. Chronic low level exposure was initially estimated to range from 160 to 320 mg/m³. Mortality due to leukaemia increased significantly. Occupational exposure to low levels (0.6 to 40 mg/m³) caused chromosomal abnormalities (Sarto et al., 1984). Furthermore, an immunotoxic action has been shown in occupationally exposed men (Mosczyński, 1981).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aidenberg and Slob, is 2,400 µg/l, the NC is 24 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 9.5 mg/kg. The NC is 0.095 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 9.5 mg/kg and 0.095 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value of 4.7 mg/m³ for rats, the

extrapolated MPC_{eco} is determined as 0.47 mg/m^3 (Rademaker et al., 1993).

For benzene it is decided to use a non-threshold approach for deriving an MPC_{human} . The MPC for humans is based on the epidemiological study of Rinsky et al. (1981) using a linear extrapolation model. In the calculation of the concentration corresponding to the accepted cancer risk of 10^{-6} per year, the assumption is made that the incidence of leukaemia resulting from exposure to equal doses by inhalation and by ingestion, is the same. The calculated MPC for humans is $0.12 \text{ } \mu\text{g/m}^3$ (Slooff, 1988). The National Health Council agreed with the conclusions of Slooff. However, the National Health Council are also of the opinion that the derived MPC is an overestimation of the risk due to Slooff's use of a linear extrapolation model. Thus the MPC for humans is set at $12 \text{ } \mu\text{g/m}^3$ (National Health Council, 1987).

Since the MPC_{human} is lower than the MPC_{eco} , the MPC in air is set at $12 \text{ } \mu\text{g/m}^3$. The NC is $0.12 \text{ } \mu\text{g/m}^3$ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	2,400	9.5	9.5	12
NC	24	0.095	0.095	0.12

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. As a result, the harmonization procedure is carried out in two possible situations: that is emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Based on this calculation the steady-state concentration in air is 16 times higher than the MPC in air. Therefore the MPC in surface water must be adjusted downwards. Using an adjustment factor of 10, the harmonized MPC in surface water is calculated to be $240 \text{ } \mu\text{g/l}$. The harmonized NC is $2.4 \text{ } \mu\text{g/l}$. Consequently, the MPCs in soil and sediment are recalculated using the equilibrium partition method (Van de Plassche and Bockting, 1993). In table 3 an overview of the harmonized MPCs and NCs is given.

Table 3: Overview of harmonized Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs)

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	240	0.95	0.95	$12^{1)}$
NC	2.4	0.0095	0.0095	$0.12^{2)}$

1) the official limit value is $10 \text{ } \mu\text{g/m}^3$

2) the official target value is $1 \text{ } \mu\text{g/m}^3$

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1,2-DICHLOROBENZENE

1. Introduction

1,2-Dichlorobenzene is a neutral, colourless, highly volatile liquid. It is one of the three isomers of dichlorobenzene. It is used as an intermediate product in organic synthesis. The raw material is a starting product for a number of important herbicides and for an antimicrobial agent which is contained in deodorant soaps (GDCh, 1990^b). In addition, the compound is used as a solvent for the manufacturing of isocyanates. For the derivation of harmonized MPCs and NCs the bioaccumulation potential of 1,2-dichlorobenzene has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 95-50-1
Molecular formula : C₆H₄Cl₂

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2-dichlorobenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
147.01	0.070	3.43	22	22	0.40	No	0.196

MW = molecular weight (in g/mol)
K_{aw} = air-water partition coefficient
K_{ow} = octanol-water partition coefficient
Kp = partition coefficient (in l/kg)
k_{deg} = degradation rate constant in air (in 10⁻⁶/s)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data are available on algae, crustaceans and fish. Chronic data are only available on crustaceans. For marine organisms, acute data are available on crustaceans and fish and chronic data on algae and molluscs (part II; appendix A). The lowest NOEC is 185 µg/l for freshwater crustaceans (Hesse et al., 1991).

Because the effects of 1,2-dichlorobenzene can be narcotic, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco}, only acute data on mice and rats are available (part II; appendix A). All data are from one taxonomic group, namely mammals. The lowest LC₅₀ is 1,890 mg/m³ (DCV) for mice (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Documents on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

Exposure of rats, guinea pigs, rabbits and monkeys at a concentration of 560 mg/m³ for 7 hours per day, 5 days per week up to 7 months, did not result in adverse effects. In addition, exposure of rats, guinea pigs and mice to 290 mg/m³ (DCV: 60.4 mg/m³) for 7 hours per day, 5 days per week for 6.5 months also resulted in no adverse effects (Hollingsworth et al., 1958; Rademaker et

week for 6.5 months also resulted in no adverse effects (Hollingsworth et al., 1958; Rademaker et al., 1993).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. The compound was negative in five of the Ames tests. In addition, the compound was found positive in a mouse micronucleus test (Mohtashamipur et al., 1987). However, it is provisionally concluded that the data are too limited to classify 1,2-dichlorobenzene as genotoxic (Hesse et al., 1991).

In a carcinogenicity study, rats and mice were given 0, 60 or 120 mg/kg body weight by stomach tube daily for 2 years (NTP, 1985⁶). Based on the results of this study it was concluded that there is no evidence that 1,2-dichlorobenzene is carcinogenic in experimental animals (Hesse et al., 1991).

Teratogenicity and reproduction

In a teratogenicity study with rats and rabbits, the highest concentration tested (2,400 mg/m³) did not result in any embryotoxic or teratogenic effects in the tested animals after an exposure for 6 hours per day, on day 6 through day 15 (rats) or day 6 through day 18 (rabbits) of gestation. In rabbits slight maternal toxicity occurred in the highest dose groups (Hesse et al., 1991).

Reproduction studies are not available (Hesse et al., 1991).

Human studies

Human studies are not available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 270 µg/l, the NC is 2.7 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all dichlorobenzene isomers, is 250 µg/l (Van de Plassche et al., 1993). The overall NC is 2.5 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 5.9 mg/kg, the NC is 0.059 mg/kg (Van de Plassche and Bockting, 1993).

However it is decided to use the MPC and NC in soil based on the data for 1,4-dichlorobenzene (Van de Plassche and Bockting, 1993) (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 5.9 mg/kg and 0.059 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all dichlorobenzene isomers, is 5.5 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.055 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value, the extrapolated MPC_{eco} is determined as 1,900 µg/m³ (Rademaker et al., 1993).

Since 1,2-dichlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the lowest corrected NOAEL of 60.4 mg/m³, so the MPC_{human} is 60 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 60 µg/m³. The NC in air is 0.60 µg/m³ (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	250	5.5	5.5	60
NC	2.5	0.055	0.055	0.60

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available, resulting in a lower uncertainty factor to be applied, a new MPC in air can be derived. For the time being, MPCs for 1,2-dichlorobenzene in water, soil and sediment are set equal to the overall MPC values calculated as the mean of MPCs for all dichlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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1,3-DICHLOROBENZENE

1. Introduction

1,3-Dichlorobenzene is a highly volatile liquid. It is one of the three isomers of dichlorobenzene. It is used exclusively as a chemical intermediate for further processing. The products arising are used for the synthesis of pesticides and insecticides, drugs and also dyes (GDCh, 1987^b). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 541-73-1

Molecular formula : C₆-H₄-Cl₂

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,3-dichlorobenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
147.01	0.095	3.53	22	22	0.72	No	0.307

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche et al., 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data are available on algae, crustaceans and fish. Chronic data are available on crustaceans and fish. For marine organisms only acute data are available on fish (part II; appendix A). The lowest NOEC is 650 µg/l for freshwater crustaceans (Hesse et al., 1991).

Because 1,3-dichlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Documents on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

(Sub)chronic toxicity data are not available (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. The compound was negative in two Ames tests. In addition, the compound was found positive in a mouse micronucleus test (Mohtashamipur et al., 1987). However, it is provisionally concluded that the data are too limited to classify 1,3-dichlorobenzene as genotoxic (Hesse et al., 1991).

Carcinogenicity studies are not available (Hesse et al., 1991).

Carcinogenicity studies are not available (Hesse et al., 1991).

Teratogenicity and reproduction

Teratogenicity and reproduction studies are not available (Hesse et al., 1991).

Human studies

Human studies are not available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 210 µg/l, the NC is 2.1 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all dichlorobenzene isomers, is 250 µg/l (Van de Plassche et al., 1993). The overall NC is 2.5 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 4.6 mg/kg, the NC is 0.046 mg/kg (Van de Plassche and Bockting, 1993).

However it is decided to use the MPC and NC in soil based on the data for 1,4-dichlorobenzene (Van de Plassche and Bockting, 1993) (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 4.6 mg/kg and 0.046 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all dichlorobenzene isomers, is 5.5 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.055 mg/kg (table 2).

3.4 Air

No MPC in air is calculated because of the lack of data (Rademaker et al., 1993; Rademaker and Van de Plassche, 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	250	0.40	5.5	-
NC	2.5	0.004	0.055	-

4. Harmonization of MPCs and NCs

The harmonization procedure is not carried out for 1,3-dichlorobenzene, because no MPC in air is available. For the time being, MPCs for 1,3-dichlorobenzene in water and sediment are set equal to the overall MPC values and the MPC in soil is set equal to the MPC derived for 1,4-dichlorobenzene (table 2) (Van de Plassche and Bockting, 1993).

1,4-DICHLOROBENZENE

1. Introduction

1,4-Dichlorobenzene is a solid. It is one of the three isomers of dichlorobenzene. It is used in toilet blocks, urinal tablets and mothballs (Slooff et al., 1991^b). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 106-46-7

Molecular formula : $C_6H_4Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,4-dichlorobenzene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
147.01	0.091	3.44	22	22	0.32	Yes	0.090

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data and chronic data are available on algae, crustaceans and fish. For marine organisms, only acute data are available on crustaceans and fish (part II; appendix A). The lowest NOEC is 122 $\mu g/l$ for freshwater fish (Hesse et al., 1991).

Because 1,4-dichlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Chronic as well as acute toxicity data are available. Acute and chronic data are available on agricultural crops. In addition, acute data are available on earthworms. The lowest LC_{50} value is 390 mg/kg in standard soil.

The lowest NOEC is 50 mg/kg in standard soil (Hesse et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco} , sub-acute as well as (sub-)chronic data for mammals are available (part II; appendix A). A sub-acute study with mice resulted in a LOAEL of 301 mg/m³ (DCV) for mortality. The chronic studies resulted in a LOAEL of 1,142 mg/m³ (DCV) for mortality for rats, guinea pigs and rabbits. The sub-acute LOAEL is used for the derivation of an MPC_{eco} : a NOAEL of 3.01 mg/m³ is calculated as LOAEL/100 (because of the exposure time (< 1 month) and the extrapolation to a NOAEL) (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Document on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

(Sub)chronic inhalation studies have been performed on rats, mice, guinea pigs and rabbits. Parameters tested were mortality, growth, (histo)pathology, biochemistry and organ weight. There was no large variation in the response of the different species (Hesse et al., 1991). The lowest NOAEL is derived from a 76 weeks study with rats and mice exposed to 450 mg/m³, 5 hours per day, 5 days per week (DCV: 67 mg/m³) (Loeser and Lichtfield, 1983).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. The compound was negative in four Ames tests and in tests on gene mutations, chromosome aberrations and sister chromatid exchanges. With regard to in-vivo testing, a few studies with negative results are available. In addition, the compound was found positive in one of two mouse micronucleus tests. However, it is provisionally concluded that the data are too limited to classify 1,4-dichlorobenzene as genotoxic (Hesse et al., 1991).

In a carcinogenicity study, rats and mice were given 0, 150 or 300 and 600 mg/kg body weight respectively by stomach tube daily for 2 years. A significant increase in the incidence of renal tumours was observed in male rats given 300 mg/kg body weight. This increase was associated with 1,4-dichlorobenzene induced alpha-2-globulin-induced nephropathy; a condition which is extremely specific to male rats. Furthermore, mice showed a significantly increased incidence of liver tumours, which also occur naturally in the mouse strain used (NTP, 1987). From this study it was concluded that there is limited evidence to suggest that 1,4-dichlorobenzene is carcinogenic in experimental animals (Slooff et al., 1991^b).

Teratogenicity and reproduction

In a teratogenicity study with rabbits, the highest concentration tested (4,800 mg/m³) did not result in any embryotoxic or teratogenic effects (Hesse et al., 1991).

Reproduction studies are not available (Hesse et al., 1991).

Human studies

Workers exposed to concentrations ranging from 481-962 mg/m³ experienced painful eyes and nose irritations (Hollingsworth et al., 1956). A number of case reports of exposure to 1,4-dichlorobenzene showed effects on the liver, blood, central nervous system and respiratory system (Slooff et al., 1991^b).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 260 µg/l, the NC is 2.6 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all dichlorobenzene isomers, is 250 µg/l (Van de Plassche et al., 1993). The overall NC is 2.5 µg/l (table 2).

3.2 Soil

Based on the single LC₅₀ value (390 mg/kg), an MPC in soil is derived using the modified EPA method. By applying an assessment factor of 1,000, an MPC of 0.4 mg/kg is determined (Van de Plassche and Bockting, 1993). The NC is 0.0040 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 5.7 mg/kg and 0.057 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all dichlorobenzene isomers, is 5.5 mg/kg (van de Plassche and Bockting, 1993). The overall NC is 0.055 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOEC value, the extrapolated MPC_{eco} is determined as 300 µg/m³ (Rademaker et al., 1993).

Since 1,4-dichlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 100 to the lowest corrected NOAEL of 67 mg/m³, resulting in an MPC_{human} of 670 µg/m³.

Even though the MPC_{human} is higher than the MPC_{eco}, the MPC in air is set at 670 µg/m³, because of the great uncertainties in the modified EPA method used for the calculation of the MPC_{eco}, and because both values differ only by a factor 2. The NC in air is 6.7 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	250	0.40	5.5	670
NC	2.5	0.0040	0.055	6.7

4. Harmonization of MPCs and NCs

Based on the harmonization of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a definite MPC in air can be derived. For the time being, MPCs for 1,4-dichlorobenzene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all dichlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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DICHLOROPHENOLS

1. Introduction

The organic substance group, dichlorophenols, consists of the following six isomers: 2,3-dichlorophenol (2,3-DCP), 2,4-dichlorophenol (2,4-DCP), 2,5-dichlorophenol (2,5-DCP), 2,6-dichlorophenol (2,6-DCP), 3,4-dichlorophenol (3,4-DCP) and 3,5-dichlorophenol (3,5-DCP). The most important application of dichlorophenols is as an intermediary for 2,4-D and for higher chlorinated phenols. However in the Netherlands these compounds are no longer used (Slooff et al., 1991). Since the toxicity of chlorophenols is assumed to be determined predominantly by the amount and not by the position of chloro-atoms, the toxicity of all dichlorophenols is considered more or less the same. Therefore the MPC in water is set equal to the estimated MPC value for all dichlorophenols (Janus et al., 1994). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of these compounds have not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no.	:	2,3-DCP	:	576-24-9
	:	2,4-DCP	:	120-83-2
	:	2,5-DCP	:	583-78-8
	:	2,6-DCP	:	87-65-0
	:	3,4-DCP	:	95-77-2
	:	3,5-DCP	:	591-35-5
Molecular formula	:	$C_6H_4Cl_2O$		

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for dichlorophenols (Slooff et al., 1991^a)

Substance	MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
2,3-DCP	163.01	-	3.19	-	-	-	yes	-
2,4-DCP	163.01	-	2.75	440	440	-	yes	-
2,5-DCP	163.01	-	3.20	-	-	-	yes	-
2,6-DCP	163.01	-	2.80	20	20	-	yes	-
3,4-DCP	163.01	-	3.37	15-30	15-30	-	yes	-
3,5-DCP	163.01	-	3.52	-	-	-	yes	-
all DCPs	163.01	-	3.14	22	22	-	yes	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 K_p = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The $\log K_{ow}$ for all DCP's has been calculated as a mathematical mean of the individual values. The partition coefficients (K_p s) for soil and sediment are equal. The average experimental K_p for all dichlorophenols is 22 l/kg (Van de Meent et al., 1990).

2.2 Ecotoxicity data

Surface water

Acute and/or chronic toxicity data are available only on freshwater organisms (protozoa, crustaceans, fish and green algae) for the six isomers (part II; appendix A). Most data are available for 2,4-DCP. The lowest NOEC is 290 $\mu g/l$ (2,4-DCP) for fish and the lowest LC_{50} value is 1,400 $\mu g/l$ (2,4-DCP) for crustaceans (Janus et al., 1991).

Soil/sediment

Only acute toxicity data are available on organisms (oligochaetes, plants) exposed to 2,4-DCP, 3,4-DCP and 3,5-DCP via contaminated soil (part II; appendix A). The lowest LC_{50} value is 265, 221 and 160 mg/kg for 2,4-DCP, 3,4-DCP and 3,5-DCP, respectively (Janus et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Janus et al., 1991).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. This MPC is 31, 14, 2.8, 34, 1.1 and 1.8 µg/l for 2,3-DCP, 2,4-DCP, 2,5-DCP, 2,6-DCP, 3,4-DCP and 3,5-DCP, respectively. Considering the range of MPCs for dichlorophenols and the amount of toxicity data on which the MPC per compound is based, the final MPC for all dichlorophenols is estimated to be 15 µg/l. The NC is 0.15 µg/l (table 2) (Janus et al., 1994).

3.2 Soil

To derive an MPC in soil the modified EPA method is used, applying a factor of 1,000 on the lowest LC₅₀ values. This MPC is 0.26, 0.22, 0.16 mg/kg for 2,4-DCP, 3,4-DCP and 3,5-DCP, respectively. Considering the range of MPCs for dichlorophenols and the amount of toxicity data on which the MPC per compound is based, the final MPC for all dichlorophenols is estimated to be 0.20 mg/kg. The NC is 0.0020 mg/kg (table 2) (Janus et al., 1994).

3.3 Sediment

No toxicity data are available for sediment dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). This MPC is 0.33 mg/kg. The NC is 3.3*10⁻³ mg/kg (table 2) (Janus et al., 1994; Van de Meent et al., 1990).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	15	0.20	0.33	-
NC	0.15	0.0020	3.3*10 ⁻³	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.33 mg/kg) is higher than the MPC in soil based on toxicity data (table 2). Therefore the MPC in soil based on toxicity data is not adjusted downwards. The MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

ETHYLBENZENE

1. Introduction

Ethylbenzene is a volatile liquid. It is used primarily in the production of styrene. Other uses of the compound include use as a solvent, as a constituent of asphalt and of naphta and in fuels (ATSDR[®], 1990). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 100-41-4

Molecular formula : C₈H₁₀

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for ethylbenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
106.16	0.140	3.15	8.3	8.3	7.50	No	0.933

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms. For freshwater organisms, acute data are available for green algae, crustaceans and fish. Chronic data are available for bacteria, blue and green algae and protozoans. For marine organisms, only acute data are available for crustaceans and fish (part II; appendix A). The lowest NOEC is 1 mg/l for freshwater green algae (Van de Plassche et al., 1993).

Since ethylbenzene has narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, toxicity data are available for rats, rabbits and guinea pigs (part II; appendix A). The only available LC₅₀ is 2,900 mg/m³ (DCV) for rats. The lowest NOAEL is 363 mg/m³ (DCV) for growth in a study with guinea pigs (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Subchronic studies were performed in mice, rats and guinea pigs and resulted in NOAELs varying from 220 to 5,420 mg/m³. The lowest NOAEL of 39 mg/m³ (DCV), based on biochemical effect studies, was obtained from a 16-week study with rats, exposed for 5 days per week and 6 hours per day (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

Mutagenicity data are not presented. Data on carcinogenicity are not available (Rademaker and Van de Plassche, 1993).

Teratogenicity and reproduction

Teratogenicity studies are available on rats and rabbits, both being exposed for 7 hours per day. The rats were exposed during day 1 through day 19 of gestation, the rabbits from day 1 through day 24 of gestation. The NOEL is 4,300 mg/m³ (DCV: 1,254 mg/m³) (Rademaker et al., 1993). Reproduction data are not available (Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker and Van de Plassche, 1993).

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 370 µg/l, the NC is 3.7 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 3.1 mg/kg, the NC is 0.031 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 3.1 mg/kg and 0.031 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the LC₅₀ value for rats, the extrapolated MPC_{eco} is determined as 2,900 µg/m³ (Rademaker et al., 1993).

The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the NOAEL of 39 mg/m³ of a subchronic rat study, resulting in an MPC_{human} of 39 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 39 µg/m³ (Rademaker et al., 1993). The NC in air is 0.39 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	370	3.1	3.1	39
NC	3.7	0.031	0.031	0.39

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived (table 2) (Van de Plassche and Bockting, 1993).

HEXACHLOROBENZENE

1. Introduction

Hexachlorobenzene is an organic solid, which is used, amongst others, as a fungicide (as a wood preserving agent) and in the production of pentachlorophenol (Hesse et al., 1991). Hexachlorobenzene has the potential to bioaccumulate. For deriving MPCs secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 118-74-1

Molecular formula : C_6Cl_6

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for hexachlorobenzene (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
284.76	-	5.73	550	550	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 19 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are only available for freshwater organisms. Acute data are available on algae, crustaceans and fish. Chronic data are available on these species as well as on polychaeta (part II; appendix A). The lowest NOEC is $1.8 \mu g/l$ for crustaceans (Hesse et al., 1991). Because hexachlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR-approach (Van de Plassche, 1994).

Soil/sediment

Only one chronic toxicity value of 100 mg/kg is available for plants (part II; appendix A) (Hesse et al., 1991). No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Several NOECs are available for mammals, while only one is present for birds (part II; appendix A). The lowest NOEC is 0.5 mg/kg food for mammals (Van de Plassche, 1994).

The geometric mean whole body BCF for freshwater and marine water fish is 18,000 l/kg (with a maximum BCF of 22,000 l/kg) (part II; appendix A). The calculated BCF (formula 10) is 26,000 l/kg. Experimental BCFs on bivalves are not available.

The calculated BCF for bivalves is 7,000 l/kg (formula 11). For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Document on chlorobenzenes (Slooff et al., 1991^b).

(Sub)chronic toxicity

No (sub)chronic inhalation studies were described. However, (sub)chronic oral studies were performed on five species. Parameters tested were mortality, (histo)pathology, organ weight, biochemistry and reproduction. The most critical study concerned a 12-month rat study with a NOAEL on (histo)pathology of 0.05 mg/kg body weight (Slooff et al., 1991^b).

Mutagenicity and carcinogenicity

No suitable mutagenicity and carcinogenicity studies are available (Slooff et al., 1991^b).

Teratogenicity and reproduction

Teratogenicity and reproduction studies are not available (Slooff et al., 1991^b).

Human studies

No suitable human studies are available (Slooff et al., 1991^b).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 2.4 µg/l (Van de Plassche, 1994).

Indirect effects

Combining data sets for birds and mammals and applying the method of Aldenberg and Slob, reveals a NEC of 0.12 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 0.0021 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning, using the geometric mean BCF, is considerably lower than the MPC in water based on direct effects, indicating that there may well be a risk for secondary poisoning via the aquatic route. So, the final MPC for the aquatic environment is set at 0.0021 µg/l (Van de Plassche, 1994). The NC in surface water is $2.1 \cdot 10^{-5}$ µg/l (table 2).

3.2 Soil

Direct effects

To derive an MPC in soil based on direct effects, the equilibrium partitioning method is used (formula 7). The MPC is 1.3 mg/kg in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals and calculated according to the method of Aldenberg and Slob (using the BCF for earthworms) is 0.028 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is lower than the MPC in soil based on direct effects. Therefore, based on possible adverse effects due to secondary poisoning, the final MPC in soil is set at 0.028 mg/kg (Van de Plassche, 1994). The NC in soil is $2.8 \cdot 10^{-4}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore an MPC of 0.0012 mg/kg is calculated using the equilibrium partitioning method (formula 6) (Van de Plassche, 1994). The NC in sediment is $1.2 \cdot 10^{-5}$ mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data cannot be derived because of the lack of the latter (Rademaker et al., 1993).

Since hexachlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by converting the oral dose (0.050 mg/kg body weight) to an inhalation dose (0.23 mg/m³). Next, an uncertainty factor (UF) of 100 is applied resulting in an MPC_{human} of 2.3 µg/m³. Because no MPC_{eco} is derived, the MPC in air is set equal to the MPC_{human}, being 2.3 µg/m³. The NC in air is 0.023 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	0.0021	0.028	0.0012	2.3
NC	2.1*10 ⁻⁵	2.8*10 ⁻⁴	1.2*10 ⁻⁵	0.023

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs can now be considered as a coherent set of values. From the harmonization of the MPC in surface water with the MPC in soil, it can be concluded that the MPC in soil calculated by equilibrium partitioning (i.e. 0.0012 mg/kg) is lower than the MPC in soil based on toxicity data, being 0.028 mg/kg (table 2). It is decided to set the harmonized MPC in soil equal to 0.028 mg/kg (table 2) (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 1.2 µg/m³ and 0.2 µg/l, respectively (Ministry of VROM, 1997). These values are below the MPC_{air} in table 2. In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	0.0021	0.028	0.0012	2.3
NC	2.1*10 ⁻⁵	2.8*10 ⁻⁴	1.2*10 ⁻⁵	0.023
CritConc	-	-	-	1.2 (air) 0.2 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is µg/l

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MONOCHLOROBENZENE

1. Introduction

Monochlorobenzene is a highly volatile liquid. The compound is used as raw material in the pesticide and pharmaceutical industry. In addition, monochlorobenzene is used as a solvent for the manufacturing of isocyanates, oils, fats, waxes, resins, rubber and ethyl cellulose (GDCh, 1990^o).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 108-90-7

Molecular formula : C₆H₅-Cl

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for monochlorobenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	K _{deg}	Readily biodegradable	Vp
112.57	0.105	2.9	11	11	0.94	Yes	1.58

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

K_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22.

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data are available on algae, crustaceans and fish. Chronic data are available on crustaceans and fish. For marine organisms, acute data are available on algae and fish and chronic data only on algae (part II; appendix A). The lowest NOEC is 0.32 mg/l for crustaceans (Hesse et al., 1991). Because monochlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco}, only acute data on mice and rats are available (part II; appendix A). All data are from one taxonomic group, namely mammals. The lowest LC₅₀ is 1,854 mg/m³ (DCV) for mice (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are based on the Integrated Criteria Documents on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

Subchronic studies were performed on three test animals (rats, rabbits and guinea pigs), all exposed for 6 or 7 hours per day, 5 days per week. Parameters tested were haematology, biochemistry, (histo)pathology and organ weight. Corrected NOAELs varied from 42 to 195 mg/m³. The lowest corrected NOAEL is 42 mg/m³ (DCV) on (histo)pathology for the rats (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. Monochlorobenzene was negative in Ames tests (Hesse et al., 1991) and in a chromosome aberration test (Sofuni et al., 1985). The compound was questionably negative in a mouse lymphoma test (McGregor et al., 1988). In addition the compound was found positive in a mouse micronucleus test (Mohtashamipur et al., 1987). However, it is provisionally concluded that the data are too limited to classify monochlorobenzene as genotoxic (Hesse et al., 1991).

In a carcinogenicity study, rats and mice were given 0, 60 or 120 and 0, 30 or 60 mg/kg body weight respectively, by stomach tube daily for 2 years. Only in the male rats given 120 mg/kg body weight, was a significant increase in neoplastic liver nodules observed. From this study it was concluded that there is no evidence that the compound is carcinogenic in experimental animals (Hesse et al., 1991).

Teratogenicity and reproduction

In a teratogenicity study with rats and rabbits, the highest concentration tested (2,715 mg/m³) did not result in any embryotoxic or teratogenic effects in rabbits. In rats, a dose of 2,170 mg/m³ was slightly maternally toxic (Hesse et al., 1991).

In a two-generation reproduction study with rats, inhalation of up to 2,070 mg/m³ in air did not have any adverse effects on reproduction or fertility (Hesse et al., 1991).

Human studies

Human studies are not available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 690 µg/l, the NC is 6.9 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 7.6 mg/kg, the NC is 0.076 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 7.6 mg/kg and 0.076 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value, the extrapolated MPC_{eco} is determined as 1,900 µg/m³ (Rademaker et al., 1993).

Since monochlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the lowest corrected NOAEL of 42 mg/m³, resulting in an MPC_{human} of 42 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 42 µg/m³. The NC in air is 0.42 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	690	7.6	7.6	42
NC	6.9	0.076	0.076	0.42

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived.

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MONOCHLOROPHENOLS

1. Introduction

The organic substance group, monochlorophenols, consists of the following three isomers: 2-monochlorophenol (2-MCP), 3-monochlorophenol (3-MCP) and 4-monochlorophenol (4-MCP). The most important application of monochlorophenols is as an intermediary for higher chlorinated phenols. However in the Netherlands these compounds are no longer used (Slooff et al., 1991). Since the toxicity of chlorophenols is assumed to be determined predominantly by the amount and not by the position of chloro-atoms, the toxicity of all monochlorophenols is considered more or less the same. Therefore the MPC in water is set equal to the estimated MPC value for all monochlorophenols (Janus et al., 1994).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no.	:	2-MCP	:	95-57-8
	:	3-MCP	:	108-43-0
	:	4-MCP	:	106-48-9
Molecular formula	:	C_6H_5ClO		

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for monochlorophenols (Slooff et al., 1991^a)

Substance	MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
2-MCP	128.56	-	2.2	-	-	-	yes	-
3-MCP	128.56	-	2.5	6-12	6-12	-	yes	-
4-MCP	128.56	-	2.6	-	-	-	yes	-
all MCPs	128.56	-	2.42	9	9	-	yes	-

MW	=	molecular weight (in g/mol)
K_{aw}	=	air-water partition coefficient
K_{ow}	=	octanol-water partition coefficient
K_p	=	partition coefficient (in l/kg)
k_{deg}	=	degradation rate constant in air (in $10^{-6}/s$)
Vp	=	vapour pressure (in kPa)

The $\log K_{ow}$ for all MCPs has been calculated as a mathematical mean of the individual values. The partition coefficients (K_p) for soil and sediment are equal. The average experimental K_p for all monochlorophenols is 9 l/kg (Van de Meent et al., 1990).

2.2 Ecotoxicity data

Surface water

Acute and/or chronic toxicity data are available only on freshwater organisms (protozoa, green algae, crustaceans and fish) for all three isomers (part II; appendix A). Most data are available on acute toxicity for 2-MCP and 4-MCP. The lowest NOEC is 500 $\mu g/l$ (2-MCP) and the lowest LC_{50} value is 2,500 $\mu g/l$ (4-MCP), both for crustaceans (Janus et al., 1991).

Soil/sediment

Only acute toxicity data are available on organisms (oligochaetes, plants) exposed to 2-MCP or 3-MCP via contaminated soil (part II; appendix A). The lowest LC_{50} value is 213 mg/kg (3-MCP) (Janus et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Janus et al., 1991).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method applying a factor of 100 or 1,000 on the lowest LC_{50} for each isomer. This MPC is 26, 5.5 and 25 $\mu\text{g/l}$ for 2-MCP, 3-MCP and 4-MCP, respectively. Considering the range of MPCs for monochlorophenols and the amount of toxicity data on which the MPC per compound is based, the final MPC for all monochlorophenols is estimated to be 25 $\mu\text{g/l}$. The NC is 0.25 $\mu\text{g/l}$ (table 2) (Janus et al., 1994).

3.2 Soil

To derive an MPC in soil the modified EPA method is used, applying a factor of 1,000 on the lowest LC_{50} value available for 2-MCP and 3-MCP. This MPC is 0.21 mg/kg for 2-MCP and 0.35 mg/kg for 3-MCP. Considering the range of MPCs for monochlorophenols and the amount of toxicity data on which the MPC per compound is based, the final MPC for all monochlorophenols is estimated to be 0.20 mg/kg. The NC is 0.002 mg/kg (table 2) (Janus et al., 1994).

3.3 Sediment

No toxicity data are present for sediment dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). This MPC is 0.22 mg/kg. The NC is $2.2 \cdot 10^{-3}$ mg/kg (table 2) (Janus et al., 1994; Van de Meent et al., 1990).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	25	0.20	0.22	-
NC	0.25	0.002	$2.2 \cdot 10^{-3}$	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.22 mg/kg) is higher than the MPC in soil based on toxicity data (table 2). Therefore the MPC in soil based on toxicity data is not adjusted downwards. The MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

2-MONOCHLOROTOLUENE

1. Introduction

2-Monochlorotoluene is a volatile liquid. It is used as an intermediate in the production of organic substances. It can also be used as a solvent (GDCh, 1989^c). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 95-49-8

Molecular formula : C₇-H₇-Cl

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 2-monochlorotoluene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
126.58	0.206	3.32	105	105	2.00	No	0.36

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms. For freshwater organisms acute data are available for crustaceans and chronic data also for bacteria, blue and green algae. For marine organisms only acute data are available for crustaceans and fish (part II; appendix A). The lowest LC₅₀ is 7.8 mg/l for marine fish. The lowest NOEC is 0.21 mg/l for freshwater crustaceans (Van de Plassche et al., 1993).

Since 2-monochlorotoluene has narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, only limited information on rats is available (part II; appendix A). A NOAEL of 46.9 mg/m³ (DCV) for growth for rats is obtained by dividing the value presented in the appendix by 10 because the exposure time was less than 1 month (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

No suitable (sub)chronic toxicity studies are available (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

No mutagenicity or carcinogenicity data are available (Rademaker et al., 1993).

Teratogenicity and reproduction

A teratogenicity study in rats exposed from day 6 through day 19 of gestation resulted in a NOAEL on reproduction of 775 mg/m³ (DCV).

Other reproduction data are not available (Rademaker et al., 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 300 µg/l, the NC is 3 µg/l. The overall MPC, calculated as the mean of MPCs for all monochlorotoluene isomers, is 310 µg/l (Van de Plassche et al., 1993). The overall NC is 3.1 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 31 mg/kg, the NC is 0.31 mg/kg.

The overall MPC, calculated as the mean of MPCs for all monochlorotoluene isomers, is 33 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.33 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC in sediment is equal to the MPC in soil, being 31 mg/kg. The NC is 0.31 mg/kg.

The overall MPC, calculated as the mean of MPCs for all monochlorotoluene isomers, is 33 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.33 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the NOAEL value for growth for rats, the extrapolated MPC_{eco} is determined as 4,700 µg/m³ (Rademaker et al., 1993).

The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the NOAEL of 775 mg/m³ of a teratogenicity rat study, resulting in an MPC_{human} of 775 µg/m³ (780 µg/m³). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 780 µg/m³ (Rademaker et al., 1993). The NC in air is 7.8 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	310	33	33	780
NC	3.1	0.33	0.33	7.8

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 2-monochlorotoluene for water, sediment and soil are set equal to the overall MPC values, calculated as the mean of MPCs for all monochlorotoluene isomers (Van de Plassche and Bockting, 1993) (table 2).

3-MONOCHLOROTOLUENE

1. Introduction

3-Monochlorotoluene is a volatile liquid. It is used as a solvent as well as a starting product for manufacturing dyestuffs and dyeing auxiliaries (GDCh, 1989^c). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 108-41-8

Molecular formula : C₇-H₇-Cl

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 3-monochlorotoluene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
126.58	0.170	3.28	95	95	1.17	No	0.36

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only one toxicity value is available, being an LC₅₀ on marine organisms (crustacean) of 25 mg/l (part II; appendix A) (Van de Plassche et al., 1993).

Since 3-monochlorotoluene has narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, no useful (eco) toxicological data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

No useful (human) toxicity data are available.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 330 µg/l, the NC is 3.3 µg/l. The overall MPC, calculated as the mean of MPCs for all monochlorotoluene isomers, is 310 µg/l (Van de Plassche et al., 1993). The overall NC is 3.1 µg/l (table 2).

Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC

in soil is 31 mg/kg, the NC is 0.31 mg/kg.

The overall MPC, calculated as the mean of MPCs for all monochlorotoluene isomers, is 33 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.33 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC in sediment is equal to the MPC in soil, being 31 mg/kg. The NC in sediment is 0.31 mg/kg.

The overall MPC, calculated as the mean of MPCs for all monochlorotoluene isomers, is 33 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.33 mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	310	33	33	-
NC	3.1	0.33	0.33	-

4. Harmonization of MPCs and NCs

Because the equilibrium partitioning method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the equilibrium partitioning method is meaningless. For the time being, MPCs for 3-monochlorotoluene in water, sediment and soil are set equal to the overall MPC values, calculated as the mean of MPCs for all monochlorotoluene isomers (Van de Plassche and Bockting, 1993) (table 2).

4-MONOCHLOROTOLUENE

1. Introduction

4-Monochlorotoluene is a volatile liquid. It is used as an intermediate in the production of several organic substances. The compound can also be used as a solvent (GDCh, 1989^o). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 106-43-4

Molecular formula : C₇H₇Cl

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 4-monochlorotoluene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
126.58	0.208	3.33	110	110	2.46	No	0.31

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms. For freshwater organisms, acute data are available on crustaceans and chronic data also on fish. For marine organisms only acute data are available on crustaceans (part II; appendix A). The lowest NOEC is 0.32 mg/l for freshwater crustaceans (Van de Plassche et al., 1993).

Since 4-monochlorotoluene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, no useful (eco) toxicological data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

For 4-monochlorotoluene no useful (human) toxicity data are available.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 300 µg/l. The NC is 3.0 µg/l. The overall MPC, calculated as the mean of MPCs for the monochlorotoluene isomers, is 310 µg/l (Van de Plassche et al., 1993). The overall NC is 3.1 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 32 mg/kg, the NC is 0.32 mg/kg.

The overall MPC, calculated as the mean of MPCs for the monochlorotoluene isomers, is 33 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.33 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC in sediment is equal to the MPC in soil, being 32 mg/kg. The NC is 0.32 mg/kg.

The overall MPC, calculated as the mean of MPCs for the monochlorotoluene isomers, is 33 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.33 mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	310	33	33	-
NC	3.1	0.33	0.33	-

4. Harmonization of MPCs and NCs

Because the equilibrium partitioning method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the equilibrium partitioning method is meaningless. For the time being, MPCs for 4-monochlorotoluene in water, sediment and soil are set equal to the overall MPC values, calculated as the mean of MPCs for the monochlorotoluene isomers (Van de Plassche and Bockting, 1993) (table 2).

PENTACHLOROBENZENE

1. Introduction

Pentachlorobenzene is an organic solid, which is used as a laboratory reagent and as a fungicide (CEPA, 1993^a). The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 608-93-5

Molecular formula : C₆-H-Cl₅

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for pentachlorobenzene (Van de Plassche, 1994)

MW	K _{sw}	log K _{ow}	K _{psoil}	K _{psoil}	K _{deg}	Readily biodegradable	Vp
250.32	0.013	5.18	398	398	0.72	No	0.0022

MW = molecular weight (in g/mol)

K_{as} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are only available on freshwater organisms (part II: appendix A). Acute data are available on algae, crustaceans and fish. Chronic data are only available on crustaceans and fish. The lowest NOEC is 10 µg/l for crustaceans (Hesse et al., 1991). Because pentachlorobenzene can have narcotic effects, the MPC is derived using the QSAR approach (Van de Plassche, 1994).

Soil/sediment

Toxicity data are only available on one species. The LC₅₀ value is 280 mg/kg, the NOEC value is 50 mg/kg in standard soil (part II: appendix A) (Hesse et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

No useful data are available for the derivation of an MPC_{eco} (Rademaker et al., 1993).

Secondary poisoning

No toxicity data are available for birds, while only two, almost equal values, are available for mammals (part II; appendix A). The lowest NOEC is 5 mg/kg food (Van de Plassche, 1994).

The geometric mean whole body BCF for freshwater fish is 5,300 l/kg (with a maximum BCF of 8,100 l/kg) (part II; appendix A). For marine water fish no experimental BCF is available. The calculated BCF for fish (formula 10) is 7,300 l/kg. Experimental BCFs on bivalves are not available. The calculated BCF for bivalves is 2,000 l/kg (formula 11). For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Documents on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

No (sub)chronic inhalation studies were described. However, (sub)chronic oral studies were performed on three species. Parameters tested were (histo)pathology, organ weight and reproduction. The most critical study concerned a 13-week rat study with a NOAEL on organ weight and (histo)pathology of 1.7 mg/kg body weight (Hesse et al., 1991).

Mutagenicity and carcinogenicity

The compound was negative in two Ames tests (Lawlor et al., 1979; Haworth et al., 1983). No suitable carcinogenicity studies are available (Hesse et al., 1991).

Teratogenicity and reproduction

Teratogenicity studies are not available (Hesse et al., 1991). In a rat study, suckling pups from mothers fed 250 mg/kg body weight developed tremors 4 to 14 days after birth; at a (maternal) dose of 6.3 mg/kg body weight this was not apparent (Linder et al., 1980).

Human studies

No suitable human studies are available (Slooff et al., 1991^b).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 7.5 µg/l (Van de Plassche, 1994).

Indirect effects

Since there are no chronic toxicity data available on birds, the NEC based on the combined data set is equal to the NEC for mammals. This latter NEC, based on the modified EPA method, is 0.5 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 0.030 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is a factor of 250 lower than the MPC in water based on direct effects, indicating that there might be a risk for secondary poisoning via the aquatic route. So, the final MPC for the aquatic environment is set at 0.030 µg/l (Van de Plassche, 1994). The NC in surface water is $3.0 \cdot 10^{-4}$ µg/l (table 2).

3.2 Soil

Direct effects

To derive an MPC in soil based on direct effects, the modified EPA method is used, applying a factor of 1,000 on the lowest LC₅₀. The MPC is 0.3 mg/kg in standard soil (Van de Plassche and Bockting, 1993).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals and calculated with the modified EPA method (using the BCF for earthworms) is 0.12 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is slightly lower than the MPC in soil based on direct effects. It is decided to set the final MPC in soil at 0.12 mg/kg (Van de Plassche, 1994). The NC in soil is $1.2 \cdot 10^{-3}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6) and is 0.012 mg/kg (Van de Plassche, 1994). The NC in sediment is $1.2 \cdot 10^{-4}$ mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data cannot be derived because of the lack of the latter (Rademaker et al., 1993).

Since pentachlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by converting the oral dose (1.7 mg/kg body weight) to an inhalation dose (7.9 mg/m³). Next, an uncertainty factor (UF) of 1,000 is applied, resulting in an MPC_{human} of 8.0 µg/m³. Because no MPC_{eco} is derived, the MPC in air is set equal to the MPC_{human}, being 8.0 µg/m³. The NC in air is 0.080 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	0.030	0.12	0.012	8.0
NC	$3.0 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$1.2 \cdot 10^{-4}$	0.080

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived (Van de Plassche and Bockting, 1993).

The harmonization procedure for surface water, sediment and soil is performed using the equilibrium partitioning. The MPC in soil, calculated by equilibrium partitioning (i.e. 0.012 mg/kg) is lower than the MPC in soil, based on toxicity data, being 0.12 mg/kg (table 2). Even though there is a serious lack of data (only one study with plants and two with mammals are available) it is decided that the harmonized MPC in soil should be set at 0.12 mg/kg (table 2) (Van de Plassche et al., 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 1.5 µg/m³ and 9 µg/l, respectively (Ministry of VROM, 1997). These values are below the MPC_{air} in table 2. In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	0.030	0.12	0.012	-
NC	$3.0 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$1.2 \cdot 10^{-4}$	-
CritConc	-	-	-	1.5 (air) 9 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is µg/l

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PENTACHLOROPHENOL

1. Introduction

Pentachlorophenol is an organic substance, which was formerly used as an insecticide, algicide, herbicide and fungicide (particularly in the preservation of wood and wood products). In the Netherlands, its use has been prohibited now (Slooff et al., 1991^a). The compound might have the potential to bioaccumulate. For deriving MPCs secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 87-86-5
Molecular formula : C_6HCl_5O

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for pentachlorophenol (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
-	-	4.74	87	87	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 K_p = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Many chronic toxicity data are available on freshwater and marine organisms. For freshwater organisms, data are available on bacteria, blue and green algae, plants, molluscs, crustaceans, insects, fish and amphibians. Chronic data for marine water organisms are available on algae, annelides, crustaceans and fish (part II; appendix A). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity to pentachlorophenol. The lowest NOEC available is one for freshwater molluscs: $3.2 \mu g/l$ (Emans et al., 1992; Jonkers et al., 1992; Van de Plassche, 1994).

Soil/sediment

Chronic as well as acute toxicity data are available for soil organisms: acute data for plants and oligochaetes; chronic data for plants, oligochaetes and microbial processes (part II; appendix A). The lowest NOEC is 1.6 mg/kg for plants (Janus et al., 1991; Van de Plassche, 1994). No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

No MPC in air has been derived yet. There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Only one NOEC is available for birds, while two are available for mammals (part II; appendix A). The lowest NOEC is 55 mg/kg food for mammals (Romijn et al., 1994; Van de Plassche, 1994). The geometric mean whole body BCF for freshwater and marine fish is 140 l/kg (with a maximum BCF of 770 l/kg) (part II; appendix A). The calculated BCF for fish (formula 10) is $2,600 \text{ l/kg}$. The experimental BCF for freshwater and marine bivalves is 88 l/kg (with a maximum BCF of 130 l/kg) (part II; appendix A). The calculated BCF for bivalves (formula 11) is 710 l/kg . For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC based on direct effects is derived by applying an alternative statistical method. This method is described in Van de Meent et al., 1990. The MPC is 2.0 µg/l, the NC is 0.020 µg/l (Janus et al., 1994; Van de Meent et al., 1990).

Indirect effects

The MPC, based on the combined data set for birds and mammals and calculated with the modified EPA method, using an assessment factor of 10 on the lowest NOEC, is 5.5 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC on the combined data sets of birds and mammals is 13 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is higher than the MPC in water based on direct effects. If the maximum BCF is used the opposite conclusion must be drawn. It is concluded that there probably will be no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC for the aquatic environment is set at 2.0 µg/l (Van de Plassche, 1994). The NC in surface water is 0.020 µg/l (table 2).

3.2 Soil

Direct effects

The modified EPA method is used to derive an MPC in soil based on direct effects, applying a factor of 10 on the lowest NOEC. This MPC is 0.16 mg/kg in standard soil (Janus et al., 1994; Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain based on the combined data set for birds and mammals and calculated with the modified EPA method, using the BCF for earthworms, is 1.3 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is higher than the MPC in soil based on direct effects, even if the maximum BCF is used, indicating that there is probably no risk of secondary poisoning via the terrestrial route. Thus, the final MPC in soil is set at the MPC based on direct effects on terrestrial organisms, i.e. 0.2 mg/kg (rounded off) (Janus et al., 1994; Van de Plassche, 1994). The NC in soil is 0.002 mg/kg (rounded off) (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore an MPC of 0.17 mg/kg is calculated using the equilibrium partitioning method (formula 6) (Van de Plassche, 1994). The NC in sediment is $1.7 \cdot 10^{-3}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Final Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	2.0	0.20	0.17	-
NC	0.020	0.0020	$1.7 \cdot 10^{-3}$	-

4. Harmonization of MPCs and NCs

Because only MPCs for surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC in soil calculated by equilibrium partitioning (0.17 mg/kg) is in good agreement with the MPC based on toxicity data, being 0.20 mg/kg (rounded off). It is decided that the harmonized MPC in soil should be set equal to the one based on direct effects on soil organisms, i.e. 0.20 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 1.1 $\mu\text{g/m}^3$ and 56 $\mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	2.0	0.20	0.17	-
NC	0.020	0.0020	$1.7 \cdot 10^{-3}$	-
CritConc	-	-	-	1.1 (air) 56 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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STYRENE

1. Introduction

Styrene is a colourless liquid. It is used exclusively to manufacture polymeric products and ranks among ethylene, propylene and vinylchloride as being one of the most important monomers. It is the raw material for thermoplastics, thermosets, elastomers and dispersions (GDCh, 1990^a).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 100-42-5

Molecular formula : C_8H_8

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for styrene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
104.15	0.177	2.95	45	45	10	No	0.60

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as marine organisms (part II; appendix A). For freshwater organisms acute data are available on crustaceans and fish, chronic data on bacteria, blue algae and protozoans. For marine organisms only acute data are available on crustaceans and fish. The lowest NOEC is 34 mg/l for blue algae (Van de Plassche et al., 1993). Since styrene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , (sub-)acute as well as (sub-)chronic toxicity data are available (part II; appendix A). All data are from one taxonomic group, namely mammals (mouse, rat, guinea pig, hamster, rabbit). The lowest LC_{50} is 1,890 mg/m³ (DCV) for rats. The lowest NOAEL is 26.3 mg/m³ (DCV) for reproduction for mice calculated as LOAEL/10 (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on styrene (Ministry of VROM, 1986^c).

(Sub)chronic toxicity

In a 6-month inhalation study, rats, guinea pigs, rabbits and monkeys were exposed to concentrations of 6,000 to 9,300 mg/m³ for 8 hours per day and 5 days per week. The concentration of 6,000 mg/m³ (DCV: 1,429 mg/m³) caused irritation of the eyes and the nose, and inhibition of growth in rats and guinea pigs. In some rats the liver and kidney weights were slightly increased (Spencer et al., 1942). In several studies in which rats were exposed to concentrations of 1,260 mg/m³ for 6 hours per day and 5 days per week, during 11 weeks, the following effects were observed: sleepiness, a temporary increase in the motoric nerve rate of conductivity,

biochemical changes in the brain, an increased activity of enzymes involved in the detoxification mechanism, and pathological changes in the liver (Vainio et al., 1979; Savolainen and Pfaffli, 1978; Seppalainen, 1978). Mice exposed to a concentration of 1,260 mg/m³ for 5 hours per day and 5 days per week during 6 weeks, showed microscopic changes in the lungs (Morisset et al., 1979). Because of the high exposure levels used, it was not possible to determine a concentration without effect in these tests (Ministry of VROM, 1986^c).

Mutagenicity and carcinogenicity

Styrene is mutagenic after metabolic activation in bacterial tests and in yeast (Loprieno et al., 1976^a; Vainio et al., 1976). It induces gene mutations in prokaryotic and eukaryotic micro-organisms, in *Drosophila melanogaster* (Donner et al., 1979) and in mammalian cells in vitro (Beye and Jensen, 1982). The compound also caused chromosomal abnormalities in mammalian cells in vitro (Ishidate and Yoshikawa, 1980; Linnainmaa et al., 1978). In mice and rats only at high concentrations ($\geq 1,625$ and 1,260 mg/m³, respectively) were any effects of chromosome damage detected in in-vivo tests (Connor et al., 1980; Meretoja et al., 1978).

In two inhalation studies rats were exposed to concentrations of 2,520 or 4,200 mg/m³ for 6 hours per day, 5 days per week, during 20 months (Jersey et al., 1978) and to concentrations of 105, 210, 420, 840 or 1,260 mg/m³, 4 hours per day, 5 days per week, during 52 weeks (Maltoni, 1978). No statistically significant increase in tumour incidence has been observed in these studies. For animals as well as humans there is no evidence to suggest that styrene is a carcinogenic substance (Ministry of VROM, 1986^c).

Teratogenicity and reproduction

Embryotoxic effects were observed in mice exposed to 1,050 mg/m³ for 6 hours per day, on day 6 through day 16 of gestation (Kankaanpää et al., 1980). Embryotoxic effects were also observed in rats exposed to 1,260 mg/m³ for 7 hours per day, on day 6 through day 16 of gestation (Murray et al., 1978^b). No teratogenic effects were observed.

In a 3-generation-reproduction study with rats no effects on reproduction were observed at oral dose levels of up to 21 mg/kg body weight (Litton Bionetics, 1980).

Human studies

After long-term occupational exposure the following effects were in general observed, but only at concentrations ≥ 200 mg/m³: irritation of the conjunctivae and the mucosa of the respiratory tract and pre-narcotic symptoms (Alieva et al., 1982; Harkonen, 1977; Rosen et al., 1978). In some cases neurotoxic effects on the nervous system were found (Harkonen, 1977; Rosen et al., 1978; Lorimer et al., 1978; Seppalainen, 1978). Occupational exposure to a concentration of 84 mg/m³ (time weighted average) revealed an increased frequency of some marginal effects (pre-narcotic symptoms, effects on the lower respiratory tract, and an increased gamma-glutamyltransferase-activity in the liver) (Lorimer et al., 1978).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 570 µg/l, the NC is 5.7 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 25 mg/kg, the NC is 0.25 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 25 mg/kg and 0.25 mg/kg respectively (table 2) (Van de Plassche and Bockting, 1993).

styrene

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC_{50} value of $1,890 \text{ mg/m}^3$ for rats, the extrapolated MPC_{eco} is determined as $1,900 \text{ } \mu\text{g/m}^3$ (Rademaker et al., 1993).

Since styrene is considered non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 100 to the LOAEL on pathology of 84 mg/m^3 in the long-term human study, resulting in an MPC_{human} of $800 \text{ } \mu\text{g/m}^3$. Since the MPC_{human} is lower than the MPC_{eco} , the MPC in air is set at $800 \text{ } \mu\text{g/m}^3$ (table 2) (Ministry of VROM, 1986^c; Rademaker et al., 1993; National Health Council, 1986^a). No NC for air is derived since the MPC for air was based on too limited data.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	570	25	25	800
NC	5.7	0.25	0.25	-

4. Harmonization of MPCs and NCs

In order to determine suitable emission compartments, information from literature and data from the Dutch Emission Registration have been screened. As a result, the harmonization procedure is carried out in two possible situations: emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is lower than the MPC in air, the MPC in surface water is not adjusted downwards. The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values (Van de Plassche and Bockting, 1993).

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1,2,3,4-TETRACHLOROBENZENE

1. Introduction

1,2,3,4-Tetrachlorobenzene is a solid. It is one of the three isomers of tetrachlorobenzene. The compound is used as a laboratory reagent and in the production of fungicides, herbicides, defoliants and insecticides (CEPA, 1993^c). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 634-66-2

Molecular formula : C₆H₂Cl₄

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2,3,4-tetrachlorobenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	K _{psoil}	K _{psediment}	k _{deg}	Readily biodegradable	Vp
215.88	0.013	4.64	300	300	0.30	No	0.0050

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available only for freshwater organisms. Acute data are available on algae and fish. Chronic data are available only on crustaceans (part II; appendix A). The lowest NOEC is 10 µg/l for *Daphnia magna* (Hesse et al., 1991). Because 1,2,3,4-tetrachlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Chronic as well as acute toxicity data are available. Acute and chronic data are available on agricultural crops. The lowest LC₅₀ is 160 mg/kg in standard soil. The lowest NOEC is 50 mg/kg (Hesse et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco}, no useful data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Document on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

No suitable (sub)chronic toxicity studies are available (Hesse et al., 1991; Rademaker et al., 1993).

Mutagenicity and carcinogenicity

The mutagenicity has only been examined in in-vitro tests: the compound was negative in one Ames test (Haworth et al., 1983). It is concluded that the data are too limited to suggest that this compound is genotoxic (Hesse et al., 1991).

No suitable carcinogenicity studies are available (Hesse et al., 1991).

Teratogenicity and reproduction

In a teratogenicity study, 1,2,3,4-tetrachlorobenzene was administered in daily doses of 0, 50, 100 or 200 mg/kg body weight to female rats by gavage on day 6 through day 15 of gestation. At the highest doses, a decrease in the mean number of live fetuses per litter occurred. No teratogenic effects were seen (Kacew et al., 1984; Ruddick et al., 1981).

Reproduction studies are not available (Hesse et al., 1991).

Human studies

No suitable human studies are available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 23 µg/l, the NC is 0.23 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 24 µg/l (Van de Plassche et al., 1993). The overall NC is 0.24 µg/l (table 2).

3.2 Soil

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The MPC is 0.20 mg/kg in standard soil (Hesse et al., 1991). The NC is 0.0020 mg/kg in standard soil.

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 0.072 mg/kg (Van de Plassche et al., 1993). The overall NC is 7.2*10⁻⁴ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 6.9 mg/kg and 0.069 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 7.2 mg/kg (van de Plassche and Bockting, 1993). The overall NC is 0.072 mg/kg (table 2).

3.4 Air

No MPC in air is calculated because of the lack of data (Rademaker et al., 1993). The (human) toxicity data of 1,2,4,5-tetrachlorobenzene is therefore used. The MPC_{human} of 1,2,4,5-tetrachlorobenzene is 1.6 µg/m³. Because no MPC_{eco} is derived, the MPC in air is set equal to the MPC_{human}, being 1.6 µg/m³. The NC in air is 0.016 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	24	0.072	7.2	1.6
NC	0.24	7.2*10 ⁻⁴	0.072	0.016

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 1,2,3,4-tetrachlorobenzene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all tetrachlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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1,2,3,5-TETRACHLOROBENZENE

1. Introduction

1,2,3,5-Tetrachlorobenzene is a solid. It is one of the three isomers of tetrachlorobenzene. The compound is used as a laboratory reagent and in the production of fungicides, herbicides, defoliants and insecticides (CEPA, 1993^a). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 634-90-2
Molecular formula : C₆H₂Cl₄

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2,3,5-tetrachlorobenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
215.88	0.021	4.66	300	300	0.30	No	0.010

MW = molecular weight (in g/mol)
K_{aw} = air-water partition coefficient
K_{ow} = octanol-water partition coefficient
Kp = partition coefficient (in l/kg)
k_{deg} = degradation rate constant in air (in 10⁻⁶/s)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data are available for freshwater and marine organisms. For freshwater organisms, data are available on algae, crustaceans and fish. For marine organisms data are only available for fish (part II; appendix A). The lowest LC₅₀ is 860 µg/l for *Daphnia magna* (Hesse et al., 1991).

Because 1,2,3,5-tetrachlorobenzene has narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Only acute toxicity data are available. These data are available on agricultural crops. The LC₅₀ is 6.5 mg/kg in standard soil (Hesse et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco}, no useful data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Documents on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

No suitable (sub)chronic toxicity studies are available (Hesse et al., 1991; Rademaker et al., 1993).

Mutagenicity and carcinogenicity

The mutagenicity has only been examined in in-vitro tests: 1,2,3,5-tetrachlorobenzene was negative in two Ames tests. It is concluded that the data are too limited to classify the compound as genotoxic (Hesse et al., 1991).

No suitable carcinogenicity studies are available (Hesse et al., 1991).

Teratogenicity and reproduction

In a teratogenicity study, 1,2,3,5-tetrachlorobenzene was administered in daily doses of 50, 100 or 200 mg/kg body weight to female rats by gavage on day 6 through day 15 of gestation. At the highest doses a decrease in the mean number of live fetuses per litter occurred. No teratogenic effects were seen (Kacew et al., 1984; Ruddick et al., 1981).

Reproduction studies are not available (Hesse et al., 1991).

Human studies

No suitable human studies are available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 22 µg/l, the NC is 0.22 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 24 µg/l (Van de Plassche et al., 1993). The overall NC is 0.24 µg/l (table 2).

3.2 Soil

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The indicative MPC is 0.0070 mg/kg in standard soil (Hesse et al., 1991). The NC is 7.0*10⁻⁵ mg/kg in standard soil.

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 0.072 mg/kg (Van de Plassche et al., 1993). The overall NC is 7.2*10⁻⁴ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 6.6 mg/kg and 0.066 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 7.2 mg/kg (van de Plassche and Bockting, 1993). The overall NC is 0.072 mg/kg (table 2).

3.4 Air

No MPC in air is calculated because of the lack of data (Rademaker et al., 1993). The (human) toxicity data of 1,2,4,5-tetrachlorobenzene is therefore used. The MPC_{human} of 1,2,4,5-tetrachlorobenzene is 1.6 µg/m³. Because the MPC_{eco} is not derived, the MPC in air is set equal to the MPC_{human}, being 1.6 µg/m³. The NC in air is 0.016 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	24	0.072	7.2	1.6
NC	0.24	7.2*10 ⁻⁴	0.072	0.016

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 1,2,3,5-tetrachlorobenzene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all tetrachlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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1,2,4,5-TETRACHLOROBENZENE

1. Introduction

1,2,4,5-Tetrachlorobenzene is a solid. It is one of the three isomers of tetrachlorobenzene. The compound is used as a laboratory reagent and in the production of fungicides, herbicides, defoliants and insecticides (CEPA^c, 1993). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 95-94-3

Molecular formula : C₆H₂Cl₄

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2,4,5-tetrachlorobenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	K _p _{soil}	K _p _{sediment}	k _{deg}	Readily biodegradable	Vp
215.88	0.017	4.60	300	300	0.30	No	0.0007

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater and marine organisms. For freshwater organisms, only acute data are available on algae, crustaceans and fish. For marine organisms, acute and chronic data are available for fish (part II; appendix A). The lowest NOEC is 90 µg/l for fish (Hesse et al., 1991).

Because 1,2,4,5-tetrachlorobenzene has narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Only acute toxicity data of 1,2,4,5-tetrachlorobenzene are available. These data are available on agricultural crops. The lowest LC₅₀ is 10 mg/kg in standard soil (Hesse et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco}, no useful data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Documents on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

In a 90-day study, male rats were fed diets containing 1,2,4,5-tetrachlorobenzene at levels 0, 0.034, 0.34, 3.4 and 34 mg/kg body weight. A significant increase in liver and kidney weights as well as haematological changes were seen at the highest dose. Biochemical activities were increased at diets of 3.4 and 34 mg/kg body weight. The NOEC in this study is determined as 0.34 mg/kg body weight (Chu et al., 1984).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. The compounds was negative in two Ames tests. In two studies of poor quality, an increased frequency in peripheral lymphocyte chromosomal aberrations in humans were reported. It is concluded that the data are too limited to consider 1,2,4,5-tetrachlorobenzene to be genotoxic (Hesse et al., 1991).

No suitable carcinogenicity studies are available (Hesse et al., 1991).

Teratogenicity and reproduction

In a teratogenicity study, 1,2,4,5-tetrachlorobenzene was administered daily in doses of 50, 100 or 200 mg/kg body weight to female rats by gavage on day 6 through day 15 of gestation. An increase of serum cholesterol level and aniline hydroxylase activity was observed in the 50 and 100 mg/kg body weight groups. No teratogenic effects were seen (Kacew et al., 1984; Ruddick et al., 1981).

Reproduction studies are not available (Hesse et al., 1991).

Human studies

No suitable human studies are available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 26 µg/l, the NC is 0.26 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 24 µg/l (Van de Plassche et al., 1993). The overall NC is 0.24 µg/l (table 2).

3.2 Soil

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The MPC is 0.010 mg/kg in standard soil (Hesse et al., 1991). The NC is 1.0*10⁻⁴ mg/kg in standard soil.

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 0.072 mg/kg (Van de Plassche et al., 1993). The overall NC is 7.2*10⁻⁴ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 7.8 mg/kg and 0.078 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all tetrachlorobenzene isomers, is 7.2 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.072 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data cannot be derived because no suitable data are available (Rademaker et al., 1993).

Since 1,2,4,5-tetrachlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. For the derivation of an MPC_{human} the 90-day oral rat study is used, resulting in a NOAEL on biochemistry of 0.34 mg/kg body weight. The MPC_{human} is derived by converting the oral exposure dose to an inhalation dose and subsequently applying an uncertainty factor (UF) of 1,000 to the corrected NOAEL of 1.6 mg/m³, so the MPC_{human} is 1.6 µg/m³. Because no MPC_{eco} is derived, the MPC in air is set equal to the MPC_{human}, being 1.6 µg/m³. The NC in air is 0.016 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	24	0.072	7.2	1.6
NC	0.24	$7.2 \cdot 10^{-4}$	0.072	0.016

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 1,2,4,5-tetrachlorobenzene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all tetrachlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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TETRACHLOROPHENOLS

1. Introduction

The organic substance group, tetrachlorophenols, consists of the following three isomers: 2,3,4,5-tetrachlorophenol (2,3,4,5-TeCP), 2,3,4,6-tetrachlorophenol (2,3,4,6-TeCP) and 2,3,5,6-tetrachlorophenol (2,3,5,6-TeCP). Applications of tetrachlorophenols are as a wood conservation agent and as an intermediary for pentachlorophenol. However in the Netherlands these compounds are no longer used (Slooff et al., 1991^a). Since the toxicity of chlorophenols is assumed to be determined predominantly by the amount and not by the position of chloro-atoms, the toxicity of all tetrachlorophenols is considered more or less the same. Therefore the MPC in water is set equal to the estimated MPC value for all tetrachlorophenols (Janus et al., 1994). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of these compounds has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no.	:	2,3,4,5-TeCP	:	4901-51-3
	:	2,3,4,6-TeCP	:	58-90-2
	:	2,3,5,6-TeCP	:	935-95-5
Molecular formula	:	C ₆ H ₂ Cl ₄ O		

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for tetrachlorophenols (Slooff et al., 1991^a)

Substance	MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
2,3,4,5TeCP	231.89	-	4.95	-	-	-	yes	-
2,3,4,6-TeCP	231.89	-	4.10	24/85-95	24/85-95	-	yes	-
2,3,5,6-TeCP	231.89	-	4.90	140	140	-	yes	-
all TeCPs	231.89	-	4.65	86	86	-	yes	-

MW	=	molecular weight (in g/mol)
K _{aw}	=	air-water partition coefficient
K _{ow}	=	octanol-water partition coefficient
Kp	=	partition coefficient (in l/kg)
k _{deg}	=	degradation rate constant in air (in 10 ⁻⁶ /s)
Vp	=	vapour pressure (in kPa)

The log Kow for all TeCPs has been calculated as a mathematical mean of the individual values. The partition coefficients (Kps) for soil and sediment are equal. The average experimental Kp for all tetrachlorophenols is 86 l/kg (Van de Meent et al., 1990).

2.2 Ecotoxicity data

Surface water

Toxicity data are available only on freshwater organisms for all three isomers. Only acute data are available on green algae, protozoa, crustaceans and fish. Most data are available for 2,3,4,5-TeCP (part II; appendix A). The lowest LC₅₀ value is 205 µg/l (2,3,4,5-TeCP) for fish (Janus et al., 1991).

Soil/sediment

Only acute toxicity data are available on organisms (oligochaetes) exposed to 2,3,4,5-TeCP via contaminated soil (part II; appendix A). The lowest LC₅₀ value is 272 mg/kg (Janus et al., 1991). No toxicity data are available on organisms exposed via contaminated sediment (Janus et al., 1991).

Air

There are no (eco)toxicological data to derive an MPC in air.

tetrachlorophenols

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. Considering the range of MPCs for tetrachlorophenols and the amount of toxicity data on which the MPC per compound is based, the final MPC for all tetrachlorophenols is estimated to be 1.0 µg/l. The NC is 0.010 µg/l (table 2) (Janus et al., 1994).

3.2 Soil

To derive an MPC in soil the modified EPA method is used, applying a factor of 1,000 on the lowest LC₅₀ value, only available for 2,3,4,5-TeCP. The MPC for tetrachlorophenols is based on the data for 2,3,4,5-TeCP and is 0.3 mg/kg (rounded off). The NC is 0.003 mg/kg (table 2) (Janus et al., 1994).

3.3 Sediment

No toxicity data are present for sediment dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 4). This MPC is 0.086 mg/kg. The NC is 8.6*10⁻⁴ mg/kg (table 2) (Janus et al., 1994; Van de Meent et al., 1990).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	1.0	0.3	0.086	-
NC	0.010	0.003	8.6*10 ⁻⁴	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.086 mg/kg) is lower than the MPC in soil based on toxicity data (table 2). However, since more weight is given to the MPC in soil based on toxicity data, it is decided that the harmonized MPC in soil should be set equal to the one based on toxicity data, i.e. 0.3 mg/kg. Thus the MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

TOLUENE

1. Introduction

Toluene is a colourless, volatile, inflammable liquid. Toluene is of great importance as a chemical intermediate and solvent. The use of toluene as a solvent has been increased in recent years as a result of its replacement of benzene. Other applications are the production of benzene, toluene diisocyanate, phenol, cresol, caprolactam, benzoic acid/benzaldehyde and as an additive to petrol (Slooff and Blokzijl, 1988; WHO, 1986^b).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 108-88-3

Molecular formula : C_7H_8

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for toluene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
92.14	0.164	2.79	5.7	5.7	6.20	Yes	2.93

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as marine organisms (part II; appendix A). For freshwater organisms acute data are available on crustaceans and fish. Chronic data are available on bacteria, algae and protozoa (Van der Heijden et al., 1988). For marine organisms, acute data are available on algae, crustaceans and fish. Chronic data are available on algae and fish (Van de Plassche et al., 1993). The lowest NOEC is 3.2 mg/l for marine fish. Since toluene is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Acute and chronic toxicity data are available on plants and worms (part II; appendix A). The lowest $LC_{50} > 140$ mg/kg and the lowest NOEC is 14 mg/kg both for plants (Van der Heijden et al., 1988). No toxicity data are available on organisms exposed via contaminated sediment (Slooff and Blokzijl, 1988; Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , (sub-)acute and (sub-)chronic toxicity data are available (part II; appendix A). All data are from one taxonomic group, namely mammals (mouse and rat). The lowest LC_{50} is 5,533 mg/m³ (DCV) for rats. The lowest NOAEL is 73 mg/m³ (DCV) for mortality for mice (Rademaker et al., 1993; Van der Heijden et al., 1988).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Integrated Criteria Document on toluene (Slooff and Blokzijl, 1988; Van der Heijden et al., 1988).

(Sub)chronic toxicity

Mice exposed to 15,000 mg/m³ for 3 hours per day and 5 days per week during 8 weeks showed a depression of body weight gain and an increase in liver weight (Bruckner and Peterson, 1981).

In addition, rats exposed to 7,600 or 11,300 mg/m³ for 8 hours per day during 1 or 3 weeks showed an increase in relative liver weight (Ungvary et al., 1982). In both studies no histopathological liver changes were found. Exposure of rats to 3,800 mg/m³ for 14 hours per day for 2 weeks resulted in ototoxicity (Pryor et al., 1984; Himnan, 1984). Inhalation exposure of rats to 110, 380 or 1,100 mg/m³ for 6 hours per day and 5 days per week during 24 months did not induce any histopathological changes. Slight effects on red blood cells were found at the highest dose (CIIT, 1980).

Mutagenicity and carcinogenicity

Toluene is not genotoxic in the following in-vitro test systems: bacteria, yeast and mammalian cells (Litton Bionetics, 1978; Mortelmans and Riccio, 1980; Purchase et al., 1978). Exposure to toluene vapour blocked mitosis in grasshopper embryos (Liang et al., 1983). The compound has not been demonstrated to be genotoxic in-vivo in either somatic or germ cells (EPA, 1983; Fishbein, 1985). There is no evidence that toluene has carcinogenic properties after long-term exposure in animals. No epidemiological studies on the occurrence of cancer in humans as a consequence of exposure to (exclusively) toluene are available (Van der Heijden et al., 1988).

Teratogenicity and reproduction

Fetotoxic effects were observed in mice exposed to 750 or 1,500 mg/m³ for 7 hours per day, on day 6 through day 16 of gestation (Courtney et al., 1986). Embryotoxic effects (low fetal weights) were also observed in rats continuously exposed to 1,500 mg/m³ on day 1 through day 8 of gestation (Hudak and Ungvary, 1978). In addition, embryo-lethal effects were observed in rats continuously exposed to 1,000 mg/m³ during organogenesis (Ungvary, 1985). No teratogenic effects were observed in any of these studies.

Human studies

In humans the target organ seems to be the central nervous system. Irritation of mucous membranes and effects on the central nervous system (effect on psychometric tests) cannot be excluded after exposure during 7 hours to concentrations of 375 mg/m³ or higher (Hyden et al., 1983; Baelum et al., 1985). At levels $\leq$ 150 mg/m³ no effects have been reported (Andersen et al., 1983).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 730 µg/l. The NC is 7.3 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

The MPC in soil is calculated by application of the modified EPA method and applying an assessment factor of 10 on the lowest NOEC available. The calculated MPC in soil is 1.4 mg/kg, the NC is 0.014 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC in sediment is 4.2 mg/kg and the NC is 0.042 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value of 5,533 mg/m³ for rats, the extrapolated MPC_{eco} is determined as 5,500 µg/m³ (Rademaker et al., 1993).

Since toluene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 50 to the NOAEL on pathology of 150 mg/m³ in the 7 hours human study, resulting in an MPC_{human} of 3,000 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 3,000 µg/m³ (Rademaker et al., 1993; Rademaker and Van de Plassche, 1993; Slooff and Blokzijl, 1988). The NC is 30 µg/m³ (table 2).

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3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	730	1.4	4.2	3,000
NC	7.3	0.014	0.042	30

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from literature and data from the Dutch Emission Registration have been screened. As a result, the harmonization procedure is generally carried out in two possible situations: emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is lower than the MPC in air, the MPC in surface water is not adjusted downwards. The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values (Van de Plassche and Bockting, 1993).

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1,2,3-TRICHLOROBENZENE

1. Introduction

1,2,3-Trichlorobenzene is a solid. The compound is one of the three existing isomers of trichlorobenzene. It is used in textile manufacturing and as an intermediate in the production of other chemicals (CEPA, 1993^b). For the derivation of harmonized MPCs and NCs the bioaccumulation potential has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 87-61-6

Molecular formula : $C_6H_3Cl_3$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2,3-trichlorobenzene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
181.43	0.056	4.14	100	100	0.50	No	0.028

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data and chronic data are available on algae, crustaceans and fish. For marine organisms only acute data are available on crustaceans (part II; appendix A). The lowest NOEC is 40 $\mu g/l$ for freshwater crustaceans (Hesse et al., 1991).

Because 1,2,3-trichlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Chronic as well as acute toxicity data are available. Acute and chronic data are available on agricultural crops. In addition, acute data are available on earthworms tested in four different soils. The lowest LC_{50} value is 5 mg/kg in standard soil. The lowest NOEC is also 5 mg/kg in standard soil (Hesse et al., 1991).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco} , no useful data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Document on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

No suitable (sub)chronic toxicity studies are available (Hesse et al., 1991; Rademaker et al., 1993).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. The compound was negative in one Ames test (Haworth et al., 1983) and did not increase the frequency of chromosome aberrations in chinese hamster ovary cells (Sofuni et al., 1985). With regard to in-vivo testing, one study - a mouse micronucleus test in bone marrow - found a clear positive response (Mohtashamipur et al., 1987). However, it is provisionally concluded that the data are too limited to classify the compound as genotoxic (Hesse et al., 1991).

No suitable carcinogenicity studies are available (Hesse et al., 1991).

Teratogenicity and reproduction

In a teratogenicity study female rats received 150, 300 or 600 mg/kg body weight in corn oil by gavage on day 6 through day 15 of gestation. No teratogenic or fetotoxic effects were produced. With respect to maternal toxicity the compound appeared to be toxic at 600 mg/kg body weight. (Black et al., 1988).

Reproduction studies are not available (Slooff et al., 1991^b).

Human studies

No suitable human studies are available (Slooff et al., 1991^b).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 64 µg/l, the NC is 0.64 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 67 µg/l (Van de Plassche et al., 1993). The overall NC is 0.67 µg/l (table 2).

3.2 Soil

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The MPC is 0.005 mg/kg in standard soil (Hesse et al., 1991). The NC is 5*10⁻⁵ mg/kg in standard soil.

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 0.24 mg/kg (Van de Plassche et al., 1993). The overall NC is 0.0024 mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 6.4 mg/kg and 0.064 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 6.7 mg/kg (van de Plassche and Bockting, 1993). The overall NC is 0.067 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data cannot be derived because of the lack of ecotoxicity data (Rademaker et al., 1993).

Since 1,2,3-trichlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. For the derivation of an MPC_{human} for 1,2,3-trichlorobenzene, the toxicity data of all trichlorobenzene isomers are combined. The overall MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 on the lowest corrected NOAEL of 4 mg/m³, resulting in an MPC_{human} of 4 µg/m³. Because no MPC_{eco} is derived, the MPC_{human} is set equal to the MPC_{human}, being 4.0 µg/m³. The NC in air is 0.040 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	67	0.24	6.7	4.0
NC	0.67	0.0024	0.067	0.040

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 1,2,3-trichlorobenzene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all trichlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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1,2,4-TRICHLOROBENZENE

1. Introduction

1,2,4-Trichlorobenzene is a volatile liquid. The compound is one of the three existing isomers of trichlorobenzene. It is used for further processing in the chemical industry, as a carrier in the textile industry, as a solvent and extractant (GDCh, 1987^a). For the derivation of harmonized MPCs and NCs the bioaccumulation potential has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 120-82-1
Molecular formula : C₆H₃Cl₃

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2,4-trichlorobenzene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
181.43	0.056	4.05	100	100	0.50	No	0.061

MW = molecular weight (in g/mol)
K_{aw} = air-water partition coefficient
K_{ow} = octanol-water partition coefficient
Kp = partition coefficient (in l/kg)
k_{deg} = degradation rate constant in air (in 10⁻⁶/s)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data and chronic data are available on algae, crustaceans and fish. For marine organisms only acute data are available on crustaceans and fish (part II; appendix A). The lowest NOEC is 100 µg/l for freshwater crustaceans (Hesse et al., 1991).

Because 1,2,4-trichlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Chronic as well as acute toxicity data are available. Acute and chronic data are available on agricultural crops. In addition, acute data are available on four different earthworms. The lowest LC₅₀ value is 127 mg/kg, the lowest NOEC is 50 mg/kg in standard soil (Hesse et al., 1991). No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For deriving an MPC_{eco}, no useful data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are mainly based on the Integrated Criteria Document on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

(Sub)chronic inhalation studies have been performed on rats, rabbits and monkeys. The animals were exposed to 0, 186, 370 or 742 mg/m³ 5 days per week, 7 hours per day for 26 weeks. The only compound related effects observed in these studies were transient changes in the liver and kidneys of rats. The lowest NOAEL is determined at 742 mg/m³ (DCV: 155 mg/m³) (Coate et al., 1977). In another subchronic inhalation study with rats exposed for 6 hours per day, 5 days per

week for 3 months, a NOAEL of 22.3 mg/m³ (DCV: 4 mg/m³) is determined (WHO, 1991).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. The compound was negative in three Ames tests and did not increase the frequency of chromosome aberrations in chinese hamster ovary cells (Sofuni et al., 1985). With regard to in-vivo testing, one study - a mouse micronucleus test in bone marrow - found a clear positive result (Mohtashamipur et al., 1987). However, it is provisionally concluded that the data are too limited to classify 1,2,4-trichlorobenzene as genotoxic (Hesse et al., 1991).

No suitable carcinogenicity studies are available (Hesse et al., 1991).

Teratogenicity and reproduction

In a teratogenicity study female rats were given 1,2,4-trichlorobenzene at doses of 75, 150 and 300 mg/kg body weight in corn oil by gavage on day 6 through day 15 of gestation. No teratogenic or fetotoxic effects were produced. With respect to maternal toxicity the compound appeared to be toxic at 150 mg/kg body weight (Black et al., 1988).

Reproduction studies are not available (Hesse et al., 1991).

Human studies

No suitable human studies are available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 79 µg/l, the NC is 0.79 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 67 µg/l (Van de Plassche et al., 1993). The overall NC is 0.67 µg/l (table 2).

3.2 Soil

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The MPC is 0.10 mg/kg in standard soil (Hesse et al., 1991). The NC is 0.0010 mg/kg in standard soil.

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 0.24 mg/kg (Van de Plassche et al., 1993). The overall NC is 0.0024 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 7.9 mg/kg and 0.079 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 6.7 mg/kg (van de Plassche and Bockting, 1993). The overall NC is 0.067 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data cannot be derived because of the lack of the latter (Rademaker et al., 1993).

Since 1,2,4-trichlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. For the derivation of an MPC_{human} for 1,2,4-trichlorobenzene, the toxicity data of all trichlorobenzene isomers are combined. The overall MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 on the lowest corrected NOAEL of 4 mg/m³, so the MPC_{human} is 4 µg/m³. Because no MPC_{eco} is derived, the MPC in air is set equal to the MPC_{human}, being 4.0 µg/m³. The NC in air is 0.040 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	67	0.24	6.7	4.0
NC	0.67	0.0024	0.067	0.040

4. Harmonization of MPCs and NCS

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 1,2,4-trichlorobenzene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all trichlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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1,3,5-TRICHLOROBENZENE

1. Introduction

1,3,5-Trichlorobenzene is a solid. It is one of the three existing isomers of trichlorobenzene. It is used exclusively as an intermediate in the synthesis of organic compounds (GDCh, 1989^d). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 108-70-3

Molecular formula : $C_6H_3Cl_3$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,3,5-trichlorobenzene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
181.43	0.056	4.19	100	100	0.50	No	0.028

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, only one $L(E)C_{50}$ is available of 9,070 $\mu g/l$ on algae. For marine organisms, only one NOEC is available of 1,000 $\mu g/l$ on molluscs (part II; appendix A) (Hesse et al., 1991).

Because 1,3,5-trichlorobenzene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

Chronic as well as acute toxicity data are available on agricultural crops. The lowest LC_{50} value is 615 mg/kg, the lowest NOEC is 50 mg/kg in standard soil (part II; appendix A) (Hesse et al., 1991). No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993; Hesse et al., 1991).

Air

For the derivation of an MPC_{eco} , no useful data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are based mainly on the Integrated Criteria Document on chlorobenzenes (Hesse et al., 1991; Slooff et al., 1991^b).

(Sub)chronic toxicity

(Sub)chronic inhalation studies have been performed in mice and rats. The animals were exposed at concentrations of 0, 10, 100 or 1,000 mg/m^3 for 6 hours per day, 5 days per week during 13 weeks. No changes were observed in several organs, blood or clinical parameters. The only effect that seemed treatment-related was found in the highest dose group. The lowest NOAEL is 100 mg/m^3 (DCV: 17.9 mg/m^3) (Sasmore et al., 1983).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo tests. The compound was negative in the Ames test (Haworth et al., 1983) and did not increase the frequency of chromosome aberrations in chinese hamster ovary cells (Sofuni et al., 1985). With regard to in vivo-testing, one study - a mouse micronucleus test in bone marrow - found a clear positive response (Mohtashamipur et al., 1987).

However, it is provisionally concluded that the data are too limited to suggest that 1,3,5-trichlorobenzene is genotoxic (Mohtashamipur et al., 1987).

No suitable carcinogenicity studies are available (Hesse et al., 1991).

Teratogenicity and reproduction

Teratogenicity and reproduction studies are not available (Hesse et al., 1991).

Human studies

No suitable human studies are available (Hesse et al., 1991).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 57 µg/l, the NC is 0.57 µg/l (Van de Plassche et al., 1993).

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 67 µg/l (Van de Plassche et al., 1993). The overall NC is 0.67 µg/l (table 2).

3.2 Soil

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The MPC is 0.6 mg/kg in standard soil (Hesse et al., 1991). The NC is 0.006 mg/kg.

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 0.24 mg/kg (Van de Plassche et al., 1993). The overall NC is 2.4*10⁻³ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC and NC in sediment are 5.7 mg/kg and 0.057 mg/kg, respectively (Van de Plassche and Bockting, 1993).

The overall MPC, calculated as the mean of MPCs for all trichlorobenzene isomers, is 6.7 mg/kg (van de Plassche and Bockting, 1993). The overall NC is 0.067 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data cannot be derived due to the lack of the latter (Rademaker et al., 1993).

Since 1,3,5-trichlorobenzene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. For the derivation of an MPC_{human}, the toxicity data of all trichlorobenzene isomers are combined. The overall MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 on the lowest corrected NOAEL of 4.0 mg/m³, so the MPC_{human} is 4 µg/m³. Because no MPC_{eco} is derived, the MPC in air is set equal to the MPC_{human}, being 4.0 µg/m³. The NC in air is 0.040 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	67	0.24	6.7	4.0
NC	0.67	$2.4 \cdot 10^{-3}$	0.067	0.040

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 1,3,5-trichlorobenzene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all trichlorobenzene isomers (table 2) (Van de Plassche and Bockting, 1993).

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TRICHLOROPHENOLS

1. Introduction

The organic substance group, trichlorophenols, consists of the following six isomers: 2,3,4-trichlorophenol (2,3,4-TCP), 2,3,5-trichlorophenol (2,3,5-TCP), 2,3,6-trichlorophenol (2,3,6-TCP), 2,4,5-trichlorophenol (2,4,5-TCP), 2,4,6-trichlorophenol (2,4,6-TCP) and 3,4,5-trichlorophenol (3,4,5-TCP). The most important application of trichlorophenols is as an intermediary for 2,4,5-trichlorophenoxyethanoic acid (2,4,5-T). Another use is as additive (herbicide and/or fungicide) in adhesives. In the Netherlands these compounds are used in polyvinyl acetate (PVA) adhesives (Slooff et al., 1991^a). Since the toxicity of chlorophenols is assumed to be determined predominantly by the amount and not by the position of chloro-atoms, the toxicity of all trichlorophenols is considered more or less the same. Therefore the MPC in water is set equal to the estimated MPC value for all trichlorophenols (Janus et al., 1994). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of these compounds has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no.	:	2,3,4-TCP	:	15950-66-0
	:	2,3,5-TCP	:	933-78-8
	:	2,3,6-TCP	:	933-75-5
	:	2,4,5-TCP	:	95-95-4
	:	2,4,6-TCP	:	88-06-2
	:	3,4,5-TCP	:	609-19-8
Molecular formula	:	$C_6H_3Cl_3O$		

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for trichlorophenols (Slooff et al., 1991^a)

Substance	MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
2,3,4-TCP	197.46	-	4.07	-	-	-	yes	-
2,3,5-TCP	197.46	-	4.21	-	-	-	yes	-
2,3,6-TCP	197.46	-	3.88	-	-	-	yes	-
2,4,5-TCP	197.46	-	3.72	43-78	43-78	-	yes	-
2,4,6-TCP	197.46	-	3.69	15	15	-	yes	-
3,4,5-TCP	197.46	-	4.39	24	24	-	yes	-
all TCPs	197.46	-	3.99	40	40	-	yes	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-5}/s$)
Vp = vapour pressure (in kPa)

The $\log Kow$ for all TCPs has been calculated as a mathematical mean of the individual values. The partition coefficients (Kps) for soil and sediment are equal. The average experimental Kp for all trichlorophenols is 40 l/kg (Van de Meent et al., 1990).

2.2 Ecotoxicity data

Surface water

Acute and/or chronic toxicity data are available only on freshwater organisms (protozoa, crustaceans, fish and green algae) for all isomers. Most data are available for 2,4,5-TCP and 2,4,6-TCP (part II; appendix A). The lowest LC_{50} value is 450 $\mu g/l$ (3,4,5-TCP) for crustaceans and the lowest NOEC value is 160 $\mu g/l$ (2,4,5-TCP) for fish (Janus et al., 1991).

Soil/sediment

Only acute toxicity data are available on organisms (oligochaetes, plants) exposed to 2,3,5-TCP, 2,4,5-TCP and 2,4,6-TCP via contaminated soil (part II; appendix A). The lowest LC_{50} value is 45 mg/kg for 2,3,5-TCP, 79 mg/kg for 2,4,5-TCP and 72 mg/kg for 2,4,6-TCP (Janus et al., 1991). No toxicity data are available on organisms exposed via contaminated sediment (Janus et al., 1991).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

The MPC in surface water is calculated using the modified EPA method. This MPC is 1.2, 0.6, 2.9, 0.45 and 3.2 $\mu\text{g/l}$ for 2,3,4-TCP, 2,3,5-TCP, 2,3,6-TCP, 2,4,5-TCP and 2,4,6-TCP, respectively. Considering the range of MPCs for trichlorophenols and the amount of toxicity data on which the MPC per compound is based, the final MPC for all trichlorophenols is estimated to be 2.5 $\mu\text{g/l}$. The NC is 0.025 $\mu\text{g/l}$ (table 2) (Janus et al., 1994).

3.2 Soil

To derive an MPC in soil the modified EPA method is used, applying a factor of 1,000 on the lowest LC_{50} values. This MPC is 0.04 mg/kg for 2,3,5-TCP, 0.08 mg/kg for 2,4,5-TCP and 0.72 mg/kg for 2,4,6-TCP. Considering the range of MPCs for trichlorophenols and the amount of toxicity data on which the MPC per compound is based, the final MPC for all trichlorophenols is estimated to be 0.04 mg/kg and the NC is 0.0004 mg/kg (table 2) (Janus et al., 1994).

3.3 Sediment

No toxicity data are present for sediment dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). This MPC is 0.10 mg/kg. The NC is $1.0 \cdot 10^{-4}$ mg/kg (table 2) (Janus et al., 1994; Van de Meent et al., 1990).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	2.5	0.04	0.10	-
NC	0.025	0.0004	$1.0 \cdot 10^{-4}$	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.10 mg/kg) is higher than the MPC in soil based on toxicity data (table 2). Therefore the MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

1,1,2-TRICHLOROETHANE

1. Introduction

1,1,2-Trichloroethane is a volatile liquid. The principal use of the compound is as a chemical intermediate in the production of 1,1-dichloroethene. It has also minor uses: as a solvent for the coating laid down on films and as a chemical intermediate or process solvent in pharmaceutical manufacture (IARC, 1979).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 79-00-5

Molecular formula : $C_2H_3Cl_3$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,1,2-trichloroethane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
133.39	0.017	1.89	4.9	4.9	0.33	No	3.0

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms (part II; appendix A). For freshwater organisms acute data are available on green algae, molluscs, crustaceans and fish and chronic data also on bacteria and blue algae. For marine organisms acute data are available on algae, annelides, crustaceans, molluscs and fish and chronic data on annelides, crustaceans and fish. The lowest NOEC is 3.0 mg/l for marine fish (Van de Plassche et al., 1993).

Since 1,1,2-trichloroethane can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , only acute data for mammals (mice and rats) are available. The lowest LC_{50} is 397 mg/m³ (DCV) for rats (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

No chronic or subchronic inhalation studies are available. Several subchronic and chronic oral studies are present. Tested species, rats and mice, were equally sensitive. The lowest NOAEL of 3.9 mg/kg body weight based on biochemistry, growth and hematology, was obtained from a 90-day study in mice. Converting this NOAEL value to continuous inhalation exposure results in a NOAEL of 18.2 mg/m³ (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

For 1,1,2-trichloroethane mutagenicity or carcinogenicity data are not presented (Rademaker et al., 1993).

Teratogenicity and reproduction

Teratogenicity or reproduction toxicity data are not available (Rademaker et al., 1993; Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker and Van de Plassche, 1993).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because in general more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 7,900 µg/l, the NC is 79 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 39 mg/kg, the NC is 0.39 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 39 mg/kg and 0.39 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value for rats, the extrapolated MPC_{eco} is rounded off to 400 µg/m³ (Rademaker et al., 1993).

The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the NOAEL of 18.2 mg/m³ (converted to inhalation exposure) of the oral subchronic study, resulting in an MPC_{human} of 18.2 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 18 µg/m³ (Rademaker et al., 1993). The NC in air is 0.18 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	7,900	39	39	18
NC	79	0.39	0.39	0.18

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty in the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived (Van de Plassche and Bockting, 1993).

2-XYLENE

1. Introduction

2-Xylene is a volatile liquid. It is used as an octane enhancer in gasoline and as a solvent in such products as paints, varnishes and other coatings, pesticides formulations and inks (CEPA, 1993^d). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 95-47-6

Molecular formula : C₈H₁₀

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 2-xylene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
106.16	0.123	3.12	66	66	14.7	No	0.667

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data are available on bacteria, green algae, crustaceans, insects, fish and amphibians. Chronic data are available on green algae and protozoans. For marine organisms, only acute data are available on crustaceans, echinoderms and fish (part II; appendix A). The lowest NOEC is 1 mg/l for green algae (Van de Plassche et al., 1993).

Because 2-xylene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, acute and (sub)chronic data are available (part II; appendix A). All data are from one taxonomic group, namely mammals (mouse, rat, guinea pig, rabbit, rhesus monkey, dog). The lowest LC₅₀ is 4,567 mg/m³ (DCV) for rats. The lowest NOAEL is 337 mg/m³ (DCV) for growth for rats, guinea pigs, monkeys and dogs (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Subchronic studies were performed in four test animals (rats, guinea pigs, monkeys and dogs), all exposed 24 hours per day 7 days per week. NOAELs varied from 337 to 5,075 mg/m³. The lowest corrected NOAEL (DCV) of 337 mg/m³ on growth, (histo)pathology and haematology, was the same for all mentioned animals (Rademaker et al., 1993; Rademaker and Van de Plassche, 1993).

Mutagenicity and carcinogenicity

Mutagenicity data are inconclusive. For both animals and humans only inadequate evidence on carcinogenicity is available. 2-Xylene was classified by IARC in group 3 (IARC, 1989).

Teratogenicity and reproduction

The compound was considered not teratogenic up to concentrations of 3,000 mg/m³ in the rat, exposed to 2-xylene from day 7 through day 14 of gestation, 24 hours per day (IARC, 1989). No data on reproduction toxicity are available (Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method according to Aldenberg and Slob, is 400 µg/l, the NC is 4 µg/l.

The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 380 µg/l (Van de Plassche et al., 1993). The overall NC is 3.8 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 26 mg/kg, the NC is 0.26 mg/kg.

The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 14 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.14 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 26 mg/kg and 0.26 mg/kg, respectively.

The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 14 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.14 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value, the extrapolated MPC_{eco} is determined as 4,600 µg/m³ (Rademaker et al., 1993).

Since 2-xylene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the lowest corrected NOAEL of 337 mg/m³, resulting in an MPC_{human} of 337 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 337 µg/m³ (round off to 340 µg/m³). The NC in air is 3.4 µg/m³ (table 2) (Rademaker and Van de Plassche, 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	380	14	14	340
NC	3.8	0.14	0.14	3.4

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MCPs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air.

When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 2-xylene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all xylene isomers (table 2) (Van de Plassche and Bockting, 1993).

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3-XYLENE

1. Introduction

3-Xylene is a volatile liquid. It is used as an octane enhancer in gasoline and as a solvent in such products as paints, varnishes and other coatings, pesticides formulations, inks (CEPA, 1993^d). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 108-38-3

Molecular formula : C₈-H₁₀

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 3-xylene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
106.16	0.177	3.20	16	16	24.5	No	0.80

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available for freshwater as well as marine organisms. For freshwater organisms, acute data are available on green algae, crustaceans, insects and fish. Chronic data are available on green algae and protozoans. For marine organisms only acute data are available on crustaceans and fish (part II; appendix A). The lowest NOEC is 0.7 mg/l for green algae (Van de Plassche et al., 1993).

Because 3-xylene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, some acute data are available (part II; appendix A). All data are from one taxonomic group, namely mammals (mouse, rat, rabbit). The lowest LC₅₀ is 5,728 mg/m³ (DCV) for mice. The lowest NOAEL is 300 mg/m³ (DCV) for mortality for rats, calculated as LOAEL/10 (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Reliable (sub)chronic studies are not available (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

Mutagenicity data are inconclusive. For both animals and humans only inadequate evidence on carcinogenicity is available. 3-Xylene was classified by IARC in group 3 (IARC, 1989).

Teratogenicity and reproduction

From a teratogenicity study a NOAEL of 1,000 mg/m³ on teratogenic effects was obtained in the rabbit, exposed to 3-xylene from day 7 through day 20 of gestation, 24 hours per day (IARC, 1989).

No useful data on reproduction toxicity are available (Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method according to Aldenberg and Slob, is 330 µg/l, the NC is 3.3 µg/l.

The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 380 µg/l (Van de Plassche et al., 1993). The overall NC is 3.8 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 5.2 mg/kg, the NC is 0.052 mg/kg.

The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 14 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.14 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 5.2 mg/kg and 0.052 mg/kg, respectively.

The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 14 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.14 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value, the extrapolated MPC_{eco} is determined as 5,700 µg/m³ (Rademaker et al., 1993).

Since 3-xylene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the lowest corrected NOAEL of 1,000 mg/m³, resulting in an MPC_{human} of 1,000 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 1,000 µg/m³ (Rademaker et al., 1993). The NC in air is 10 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	380	14	14	1,000
NC	3.8	0.14	0.14	10

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 3-xylene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all xylene isomers (table 2) (Van Plassche and Bockting, 1993).

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4-XYLENE

1. Introduction

4-Xylene is a volatile liquid. It is used as an octane enhancer in gasoline and as a solvent in such products as paints, varnishes and other coatings, pesticides formulations and inks (CEPA, 1993^d). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 106-42-3

Molecular formula : C₈-H₁₀

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 4-xylene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
106.16	0.181	3.15	26	26	15.2	No	0.867

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms. For freshwater organisms, acute data are available on green algae, crustaceans, insects and fish. Chronic data are available on green algae and protozoans. For marine organisms only acute data are available on crustaceans and fish (part II; appendix A). The lowest NOEC is 0.9 mg/l for green algae (Van de Plassche et al., 1993).

Because 4-xylene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, only some (sub)acute data are available (part II; appendix A). All data are from one taxonomic group, namely mammals (mouse, rat, rabbit). The lowest LC₅₀ is 3,299 mg/m³ (DCV) for rats. The lowest NOAEL is 15 mg/m³ (DCV) for reproduction for rats, calculated as LOAEL/10 (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

(Sub)chronic studies are not available (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

Mutagenicity data are inconclusive. For both animals and humans only inadequate evidence on carcinogenicity is available. 4-Xylene was classified by IARC in group 3 (IARC, 1989).

Teratogenicity and reproduction

A teratogenicity study, in which rabbits were continuously exposed for 14 days, leads to a NOAEL on teratogenicity of 1,000 mg/m³ (Rademaker and Van de Plassche, 1993; IARC, 1989). No useful data on reproduction toxicity are available (Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 400 µg/l. The NC is 4.0 µg/l. The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 380 µg/l (Van de Plassche et al., 1993). The overall NC is 3.8 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 11 mg/kg. The NC is 0.11 mg/kg. The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 14 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.14 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 11 mg/kg and 0.11 mg/kg, respectively.

The overall MPC, calculated as the mean of MPCs for all xylene isomers, is 14 mg/kg (Van de Plassche and Bockting, 1993). The overall NC is 0.14 mg/kg (table 2).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value, the extrapolated MPC_{eco} is determined as 3,300 µg/m³ (Rademaker et al., 1993).

Since 4-xylene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the lowest corrected NOAEL of 1,000 mg/m³, resulting in an MPC_{human} of 1,000 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 1,000 µg/m³ (Rademaker et al., 1993). The NC in air is 10 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	380	14	14	1,000
NC	3.8	0.14	0.14	10

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty over the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, MPCs for 4-xylene in water, soil and sediment are set equal to the overall MPC values, calculated as the mean of MPCs for all xylene isomers (table 2) (Van de Plassche and Bockting, 1993).

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APPENDIX B

POLYCYCLIC AROMATIC HYDROCARBONS

- ANTHRACENE
- BENZO(A)ANTHRACENE
- BENZO(A)PYRENE
- BENZO(K)FLUORANTHENE
- FLUORANTHENE
- NAPHTHALENE
- PHENANTHRENE

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ANTHRACENE

1. Introduction

Anthracene is one of the polycyclic aromatic hydrocarbons (PAH). It is used as an intermediate in dye production. It is also used in smoke screens, scintillation counter crystals, and organic semiconductor research. In addition, it is used to synthesize the chemotherapeutic agent, amacrine (ATSDR, 1994). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 120-12-7

Molecular formula : $C_{14}H_{10}$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for anthracene (Kalf et al., 1995)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
178.24	-	4.45	1,660	1,660	-	-	$1.0 \cdot 10^{-6}$

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal (Kalf et al., 1995).

2.2 Ecotoxicity data

Surface water

Acute and chronic toxicity data are available only on freshwater organisms (part II; appendix B). Acute data are available on fish and insects. Chronic data are available on macrophyta, algae and crustaceans. The lowest LC_{50} value is calculated as the geometric mean of 8 LC_{50} s for fish and is $6.9 \mu g/l$. The lowest NOEC is calculated as the geometric mean of 5 NOECs for crustaceans and is $1.67 \mu g/l$ (Kalf et al., 1995).

Soil/sediment

Only acute toxicity data are available on organisms exposed via contaminated soil (macrophyta) (part II; appendix B) (Kalf et al., 1995). The lowest EC_{50} is 150 mg/kg (Mitchell et al., 1988). No toxicity data are available on organisms exposed via contaminated sediment (Kalf et al., 1995).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. An assessment factor of 100 is applied on the geometric mean of 8 LC_{50} s for fish. This results in an MPC of $0.07 \mu g/l$. The NC is $0.0007 \mu g/l$ (table 2) (Kalf et al., 1995).

3.2 Soil

The MPC in soil is calculated by application of the modified EPA method and applying an assessment factor of 1,000 on the lowest EC_{50} available. This results in an MPC of 0.15 mg/kg. The MPC when calculated with the equilibrium partitioning method (formula 7) results in a value of 0.12 mg/kg. The MPC calculated with the equilibrium partitioning method is the lowest value and is used as the final MPC for soil. The NC is 0.0012 mg/kg (table 2) (Kalf et al., 1995).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Since the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil and are 0.12 mg/kg and 0.0012 mg/kg, respectively (table 2) (Kalf et al., 1995).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.07	0.12	0.12	-
NC	0.0007	0.0012	0.0012	-

4. Harmonization of MPCs and NCs

Because the equilibrium partitioning method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the equilibrium partitioning method is meaningless.

For air however, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $8.6 \mu\text{g/m}^3$ and $6.5 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.07	0.12	0.12	-
NC	0.0007	0.0012	0.0012	-
CritConc	-	-	-	8.6 (air) 6.5 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

BENZO(A)ANTHRACENE

1. Introduction

Benzo(a)anthracene is one of the polycyclic aromatic hydrocarbons (PAH). It is used as a research chemical (ATSDR, 1988^a). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 56-55-3
Molecular formula : C₁₈-H₁₂

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for benzo(a)anthracene (Kalf et al., 1995)

MW	K _{aw}	log K _{ow}	K _{p soil}	K _{p sediment}	k _{deg}	Readily biodegradable	Vp
228.30	-	5.79	36,308	36,308	-	-	2.8*10 ⁻⁸

MW = molecular weight (in g/mol)
K_{aw} = air-water partition coefficient
K_{ow} = octanol-water partition coefficient
K_p = partition coefficient (in l/kg)
k_{deg} = degradation rate constant in air (in 10⁻⁶/s)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal (Kalf et al., 1995).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms. Acute data are available on crustaceans (part II; appendix B) (Kalf et al., 1995). The lowest LC₅₀ is 10 µg/l for crustaceans (Trucco et al., 1983).

Soil/sediment

Only chronic toxicity data are available on organisms exposed via contaminated soil (crustaceans) (part II; appendix B) (Kalf et al., 1995). The lowest NOEC is 2.5 mg/kg (Van Brummelen et al., submitted). No toxicity data are available on organisms exposed via contaminated sediment (Kalf et al., 1995).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. An assessment factor of 1,000 is applied on the lowest LC₅₀ available. This results in an MPC of 0.01 µg/l. The NC is 0.0001 µg/l (table 2) (Kalf et al., 1995).

3.2 Soil

The MPC in soil is calculated using the modified EPA method. A factor 10 is applied on the lowest NOEC available. This results in an MPC of 0.25 mg/kg. The MPC when calculated with the equilibrium partitioning method (formula 7) results in a value of 0.36 mg/kg. The MPC calculated using the EPA method is the lowest value and is used as the final MPC for soil. The NC is 0.0025 mg/kg (table 2) (Kalf et al., 1995).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC in sediment is 0.36 mg/kg. The NC is 0.0036 mg/kg (table 2) (Kalf et al., 1995).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 3: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.01	0.25	0.36	-
NC	0.0001	0.0025	0.0036	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning is higher than the MPC in soil (based on toxicity data). It is therefore decided to set the harmonized MPC in soil equal to the one based on toxicity data.

For air however, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $0.2 \mu\text{g/m}^3$ and $5 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 2: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.01	0.25	0.36	-
NC	0.0001	0.0025	0.0036	-
CritConc	-	-	-	0.2 (air) 5 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

BENZO(A)PYRENE

1. Introduction

Benzo(a)pyrene is one of the polycyclic aromatic hydrocarbons (PAH). It is used as a research chemical (ATSDR, 1988^b). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 50-32-8

Molecular formula : $C_{20}H_{12}$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for benzo(a)pyrene (Kalf et al., 1995)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
252.32	-	5.97	54,954	54,954	-	-	$7.0 \cdot 10^{-10}$

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal (Kalf et al., 1995).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms. Acute data are available on algae and crustaceans. Chronic data are available on fish (part II; appendix B). The lowest LC_{50} is $5.0 \mu g/l$ for crustaceans (Trucco et al., 1983). The lowest NOEC is $6.3 \mu g/l$ (TNO, 1993).

Soil/sediment

Only chronic toxicity data are available on organisms exposed via contaminated soil (worms and crustaceans (part II; appendix B) (Kalf et al., 1995). The lowest NOEC is 2.6 mg/kg for worms (Achazi et al., 1995). No toxicity data are available on organisms exposed via contaminated sediment (Kalf et al., 1995).

Air

For the derivation of an MPC_{eco} , no useful data are available (Slooff et al., 1989).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on PAHs (Slooff et al., 1989; Montizaan et al., 1989).

(Sub)chronic toxicity

(Sub)chronic toxicity data are not available (Slooff et al., 1989).

Mutagenicity and carcinogenicity

Based on a large amount of information it is stated that benzo(a)pyrene is highly mutagenic in almost all systems (Montizaan et al., 1989).

The substance was found to be carcinogenic to mice, rats and hamsters after oral, intragastrical or intraintestinal exposure. Both local and systemic carcinogenic effects after uptake from the gastrointestinal tract were detected (Montizaan et al., 1989).

Teratogenicity and reproduction

Teratogenicity and reproduction studies are not available (Slooff et al., 1989).

Human studies

There are three sets of data available which are suited for a risk estimate for the development of lung cancer in man after occupational exposure. These studies are all suitable because smoking habits were taken into account. The first set of data concerns a prospective study investigating mortality from lung cancer in a cohort of gas workers (Pike, 1983). A second study concerns a study among Chinese house-wives who are exposure to smoky coal used for cooking in unventilated rooms (Mumford et al., 1987). The third set of data comes from a series of studies among US coke oven workers in which the observed mortality from lung cancer was very high (EPA, 1984^b).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. An assessment factor of 100 is applied on the lowest LC₅₀ available. This results in an MPC of 0.05 µg/l. The NC is 0.0005 µg/l (table 2) (Kalf et al., 1995).

3.2 Soil

The MPC in soil is calculated using the modified EPA method. A factor 10 is applied on the lowest NOEC available. This results in an MPC of 0.26 mg/kg. The NC is 0.0026 mg/kg (table 2) (Kalf et al., 1995).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). This results in an MPC of 2.7 mg/kg. The NC is 0.027 mg/kg (table 2) (Kalf et al., 1995).

3.4 Air

The MPC in air is based on toxicity data. Based on the available data, benzo(a)pyrene must be considered as a potential genotoxic carcinogen which necessitates a non-threshold approach for deriving an MPC_{human}. Thus, the MPC derived to protect humans is based on the several epidemiological studies (Montizaan et al., 1989). A value of 1 ng/m³ is calculated as an appropriate value corresponding to the accepted cancer risk of 10⁻⁶ per year (VROM, 1994; Janus et al., 1994). The MPC in air is set at the value of the MPC_{human}, being 1 ng/m³. This value is below the calculated critical concentration in air according to the Ministry of VROM (1997). The NC in air is 0.01 ng/m³ (table 2).

3.5 Overview of MPCs en NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (ng/m ³)
MPC	0.05	0.26	2.7	1.0
NC	0.0005	0.0026	0.027	0.01

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. As a result, the harmonization procedure is generally carried out in one possible situation: emission to air (Kalf et al., 1995).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Also the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to air. Because the steady-state concentrations in soil and water are lower than the calculated MPCs, the MPC in air is not adjusted downwards. The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values (Kalf et al., 1995).

BENZO(K)FLUORANTHENE

1. Introduction

Benzo(k)fluoranthene is one of the polycyclic aromatic hydrocarbons (PAH). It is used as a research chemical (ATSDR, 1994). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 205-99-2

Molecular formula : $C_{20}H_{12}$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for benzo(k)fluoranthene (Slooff et al., 1989)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
252.32	-	6.0	58,884	58,884	-	-	$5.2 \cdot 10^{-11}$

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-5}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal (Kalf et al., 1995).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms. Chronic data are available on fish (part II, appendix B) (Hooftman and Evers-de Ruijter, 1992). The lowest NOEC is calculated as the geometric mean of 2 NOECs and is $0.36 \mu g/l$ (Kalf et al., 1995).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Kalf et al., 1995).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. An assessment factor of 10 is applied on the geometric mean of 2 NOECs for fish. This results in an MPC of $0.04 \mu g/l$. The NC is $0.0004 \mu g/l$ (table 2) (Kalf et al., 1995).

3.2 Soil

Since no toxicity data are available for soil organisms, the MPC is calculated using the equilibrium partitioning method (formula 7) and is $2.4 mg/kg$. The NC is $0.024 mg/kg$ (table 2) (Kalf et al., 1995).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Since the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil and are 2.4 mg/kg and 0.024 mg/kg, respectively (table 2) (Kalf et al., 1995).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.04	2.4	2.4	-
NC	0.0004	0.024	0.024	-

4. Harmonization of MPCs and NCs

Because the equilibrium partitioning method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the equilibrium partitioning method is meaningless.

For air however, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 0.2 $\mu\text{g/m}^3$ and 47 $\mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.04	2.4	2.4	-
NC	0.0004	0.024	0.024	-
CritConc	-	-	-	0.2 (air) 47 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

FLUORANTHENE

1. Introduction

Fluoranthene is one of the polycyclic aromatic hydrocarbons (PAH). It is used as a lining material to protect the interior of steel and ductile-iron drinking water pipes and storage tanks (ATSDR, 1994). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 206-44-0

Molecular formula : $C_{16}H_{10}$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for fluoranthene (Kalf et al., 1995)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
202.26	-	5.16	8,511	8,511	-	-	$1.2 \cdot 10^{-6}$

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal (Kalf et al., 1995).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as marine organisms (part II; appendix B). For freshwater organisms chronic data are available on macrophyta and fish. For marine organisms acute data are available only on worms. Based on the data available, freshwater and marine organisms do not seem to differ significantly in their sensitivity to fluoranthene (Kalf et al., 1995). The lowest LC_{50} is 300 $\mu g/l$ for worms (Rossi and Neff, 1978).

Soil/sediment

For soil organisms no reliable toxicity data are available. Some acute toxicity data are available on organisms exposed via contaminated sediment. LC_{50} values for crustaceans range between 2 and 21 mg/kg and between 3 and 9 mg/kg for insects (Suedel et al. 1993). It is however not possible to use the experimental sediment toxicity data to derive an MPC for sediment, because no evaluation criteria for sediment studies exist at the moment (Kalf et al., 1995).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. An assessment factor of 1,000 is applied on the lowest LC_{50} available, which results in an MPC of 0.3 $\mu g/l$. The NC is 0.003 $\mu g/l$ (table 2) (Kalf et al., 1995).

3.2 Soil

Since no reliable toxicity data are available for soil organisms, the MPC is calculated using the equilibrium partitioning method (formula 7) and is 2.6 mg/kg. The NC is 0.026 mg/kg (table 2) (Kalf et al., 1995).

3.3 Sediment

Since the toxicity data for sediment-dwelling organisms cannot be used to derive an MPC, the MPC is calculated using the equilibrium partitioning method (formula 6). Since the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil and are 2.6 mg/kg and 0.026 mg/kg, respectively (table 2) (Kalf et al., 1995).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.30	2.6	2.6	-
NC	0.0030	0.026	0.026	-

4. Harmonization of MPCs and NCs

Because the equilibrium partitioning method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the equilibrium partitioning method is meaningless.

For air however, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 13 $\mu\text{g/m}^3$ and 54 $\mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.30	2.6	2.6	-
NC	0.0030	0.026	0.026	-
CritConc	-	-	-	13 (air) 54 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

NAPHTHALENE

1. Introduction

Naphthalene is one of the polycyclic aromatic hydrocarbons (PAH). In Western Europe it is mainly produced from coal tar. It is used in the production of phthalic acid anhydride, carbaryl (insecticide), beta naphthol, detergents, tanning agents, anti-moth agents (mothballs) and as raw material for paint (ATSDR^b, 1990; GDCh, 1989^a; Slooff et al., 1989). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 91-20-3

Molecular formula : C₁₀-H₈

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for naphthalene (Kalf et al., 1995)

MW	K _{aw}	log K _{ow}	K _p _{soil}	K _p _{sediment}	k _{deg}	Readily biodegradable	Vp
128.18	-	3.3	117	117	-	-	10.4*10 ⁻³

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal (Kalf et al., 1995).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as marine organisms (part II; appendix B). For freshwater organisms acute data are available on algae, molluscs, crustaceans, insects and fish. Chronic data are available on fish. For marine organisms acute data are available on molluscs, worms, crustaceans and fish. Chronic data are available on crustaceans and fish. Based on the data available, freshwater and marine organisms do not seem to differ significantly in their sensitivity to naphthalene (Kalf et al., 1995). The lowest LC₅₀ value is 120 µg/l for freshwater fish (Milleman et al., 1984). The lowest NOEC value is 21 µg/l for marine crustaceans (Caldwell et al., 1977).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Kalf et al., 1995).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. Combining the freshwater and marine data an assessment factor of 100 is applied on the lowest LC₅₀ value available. This results in an MPC of 1.2 µg/l. The NC is 0.012 µg/l (table 2) (Kalf et al., 1995).

3.2 Soil

Since no toxicity data are present for soil organisms, the MPC is calculated using the equilibrium partitioning method (formula 7) and is 0.14 mg/kg. The NC is 0.0014 mg/kg (table 2) (Kalf et al., 1995).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Since the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil and are 0.14 mg/kg and 0.0014 mg/kg, respectively (table 2) (Kalf et al., 1995).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	1.2	0.14	0.14	-
NC	0.012	0.0014	0.0014	-

4. Harmonization of MPCs and NCs

Because the EP method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the EP method is meaningless.

For air however, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $140 \mu\text{g/m}^3$ and $7.8 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	1.2	0.14	0.14	-
NC	0.012	0.0014	0.0014	-
CritConc	-	-	-	140 (air) 7.8 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

PHENANTHRENE

1. Introduction

Phenanthrene is one of the polycyclic aromatic hydrocarbons (PAH). It is used in the manufacture of dyestuffs and explosives and in biological research (ATSDR, 1994). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of this compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 85-01-8

Molecular formula : $C_{14}H_{10}$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for phenanthrene (Kalf et al., 1995)

MW	K_{ow}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
178.24	-	4.46	1,698	1,698	-	-	$2.0 \cdot 10^{-5}$

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal (Kalf et al., 1995).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as marine organisms (part II; appendix B). For freshwater organisms acute data are available on crustaceans and fish. Chronic data are available on macrophyta, crustaceans and fish. For marine organisms acute data are available on worms and crustaceans. Chronic data are available on crustaceans. Based on the data available, freshwater and marine organisms do not seem to differ significantly in their sensitivity to phenanthrene (Kalf et al., 1995). The lowest LC_{50} is $30 \mu g/l$ for freshwater fish (Milleman et al., 1984). The lowest NOEC is $32 \mu g/l$ for both freshwater crustaceans and fish (Hooftman and Evers-de Ruiters, 1992).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Kalf et al., 1995).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the modified EPA method. An assessment factor of 100 is applied on the lowest LC_{50} value available. This results in an MPC of $0.3 \mu g/l$. The NC is $0.003 \mu g/l$ (table 2) (Kalf et al., 1995).

3.2 Soil

Since no toxicity data are present for soil organisms, the MPC is calculated using the equilibrium partitioning method (formula 7) and is 0.51 mg/kg. The NC is 0.0051 mg/kg (table 2) (Kalf et al., 1995).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 4). Since the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil and are 0.51 mg/kg and 0.0051 mg/kg, respectively (table 2) (Kalf et al., 1995).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.30	0.51	0.51	-
NC	0.0030	0.0051	0.0051	-

4. Harmonization of MPCs and NCs

Because the EP method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the EP method is meaningless.

For air however, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 33 $\mu\text{g/m}^3$ and 28 $\mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.30	0.51	0.51	-
NC	0.0030	0.0051	0.0051	-
CritConc	-	-	-	33 (air) 28 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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APPENDIX C

ALIPHATIC HYDROCARBONS

- ACRYLONITRILE
- 2-CHLORO-1,3-BUTADIENE
- 3-CHLOROPROPENE
- 1,1-DICHLOROETHANE
- 1,2-DICHLOROETHANE
- 1,1-DICHLOROETHENE
- 1,2-DICHLOROETHENE
- DICHLOROMETHANE
- 1,2-DICHLOROPROPANE
- 1,3-DICHLOROPROPANE
- 1,3-DICHLOROPROPENE
- 2,3-DICHLOROPROPENE
- ETHYLENE
- ETHYLENE OXIDE
- HEXACHLOROETHANE
- PENTACHLOROETHANE
- 1,1,2,2-TETRACHLOROETHANE
- TETRACHLOROETHENE
- TETRACHLOROMETHANE
- 1,1,1-TRICHLOROETHANE

- 1,1,2-TRICHLOROETHANE
- TRICHLOROETHENE
- TRICHLOROMETHANE
- VINYLCHLORIDE

ACRYLONITRILE

1. Introduction

Acrylonitrile is a colourless and flammable liquid, mainly used for the production of polymers and copolymers in the Netherlands.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 107-13-1

Molecular formula : C_3H_3N

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for acrylonitrile (Van de Plassche et al., 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
53.06	0.002	0.25	0.089	0.089	3.4	Yes	13.3

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche et al., 1993).

2.2 Ecotoxicity data

Surface water

Acute toxicity data are available on freshwater and marine organisms (part II; appendix C). For freshwater organisms acute data are available on crustaceans and fish, for marine organisms on annelids and fish. No chronic data are available on aquatic organisms. Based on the available data, marine and freshwater organisms do not seem to differ significantly in sensitivity to acrylonitrile. The lowest LC_{50} is 7.6 mg/l for a freshwater crustacean (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on soil and sediment-dwelling organisms exposed via contaminated soil and sediment, respectively (Van de Plassche et al., 1993).

Air

Acute toxicity data are available on insects and mammals exposed via air. Chronic toxicity data are available on rats and dogs (part II; appendix C) (Van de Plassche et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on acrylonitrile (Ministry of VROM, 1984^a).

(Sub)chronic toxicity

Acrylonitrile has extensively been studied in short-term and long-term tests. In animals, short-term and long-term exposure results in respiratory changes, morphological changes in lungs, brains, liver, kidney, adrenals and gastrointestinal tract, cyanosis, convulsions and ultimately in death. Rats and rabbits exposed to 50 and 250 mg/m³ daily for a period of 6 months showed a decrease in body weight gain, increased heart weight and neuronal lesions, kidney disorders and inflammatory changes of the respiratory tracts (Knoblock et al., 1971; Krysiak and Knoblock, 1971).

Mutagenicity and carcinogenicity

The mutagenicity has been examined in in-vitro and in-vivo assays. Acrylonitrile showed positive effects in systems with bacteria (with metabolic activation) (Poncelet et al., 1980; Kawachi et al., 1980; Lyniski and Andrews, 1980), in systems with non-mammalian cells (Kawachi et al., 1980) and in-vitro mammalian systems (Kawachi et al., 1980). Negative results were obtained in in-vivo mammalian systems (Johnson et al., 1987; Leonard et al., 1981).

The lowest observable effect concentration with respect to tumour formation in a 2-year inhalation study with rats is 44 mg/m³. The rats were exposed 6 hours per day, 5 days per week. A treatment-related incidence of tumours in the central nervous systems, zymbal gland, tongue, small intestine and mammary gland were observed (Quast et al., 1980).

Teratogenicity and reproduction

In a toxicity study, rats were given 0, 10, 25 and 65 mg/kg body weight per day by gavage from day 6 through day 15 of gestation. Administration of 25 mg/kg resulted in teratogenic effects (Murray et al., 1978^a).

In a three-generation (reproduction) study with rats given 0, 100 and 500 mg/l in drinking water, effects on pup weight occurred at 100 mg/l (Beliles et al., 1980^a; EPA, 1982).

Human studies

Short-term occupational and/or accidental exposure to acrylonitrile caused local effects on skin and irritation of the mucous membranes, limb weakness, dizziness, vomiting, diarrhoea and low grade anaemia (Baxter, 1979). A reversible effect on liver and kidney-function was suggested at exposure levels > 44 mg/m³ (Wilson and McCormick, 1949). After long-term occupational exposure to 11 mg/m³ some changes in liver function tests appeared (Sakarai and Kusumoto, 1972). Epidemiological studies suggest a carcinogenic effects on humans after inhalation (O'Berg, 1980; Delzell and Monson, 1982; Thiess et al., 1981).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is derived by applying the modified EPA method. Because there are only acute toxicity data available on crustaceans and fish, an extrapolation factor of 1,000 is used. The MPC is 7.6 µg/l (Van de Plassche et al., 1993). The NC in surface water is 0.076 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on soil organisms, the MPC is calculated by means of the equilibrium partitioning method (formula 7). The MPC in soil is 6.8*10⁻⁴ mg/kg soil (Van de Plassche et al., 1993). The NC in soil is 6.8*10⁻⁶ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 6.8*10⁻⁴ mg/kg and 6.8*10⁻⁶ mg/kg, respectively (table 2) (Van de Plassche et al., 1993).

3.4 Air

The MPC in air is based on both ecotoxicity and toxicity data. The MPC in air based on ecotoxicity data is derived using the modified EPA method. The derived MPC_{eco} is based on a comparison between the lowest extrapolated acute value (230 µg/m³) and the lowest extrapolated chronic value (800 µg/m³). Based on this comparison the MPC_{eco} is set at 0.230 mg/m³ (Rademaker et al., 1993).

Based on the available data, acrylonitrile must be considered as a potential genotoxic carcinogen which necessitates a non-threshold approach for deriving an MPC_{human}. Thus, the MPC derived to protect humans is based on the carcinogenicity study (Quast et al., 1980). A concentration of 3.7 µg/m³ is calculated corresponding to the accepted cancer risk of 10⁻⁶ per year (Ministry of VROM, 1984^a). Due to the incompleteness and uncertainties of the test results this concentration is rounded off to 10 µg/m³ (National Health Council, 1985^a).

The MPC in air is set at the value of the MPC_{human}, being 10 µg/m³ (Rademaker et al., 1993) (table 2). No NC for air is derived since the MPC for air was based on too limited data.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	7.6	6.8*10 ⁻⁴	6.8*10 ⁻⁴	10
NC	0.076	6.8*10 ⁻⁶	6.8*10 ⁻⁶	-

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche et al., 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Based on this calculation the steady-state concentration in air is lower than the MPC in air. Consequently, the mentioned MPCs and NCs in table 2 can be regarded as a coherent set of values (Van de Plassche and Bockting, 1993).

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2-CHLORO-1,3-BUTADIENE

1. Introduction

2-Chloro-1,3-butadiene is a very flammable, colourless liquid. The compound is used in the production of polychloroprene elastomers (IARC, 1979^a).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 126-99-8

Molecular formula : C_4H_5Cl

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 2-chloro-1,3-butadiene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
88.54	0.083	2.16	7.2	7.2	40.0	No	23.1

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

No toxicity data are available on freshwater or marine organisms. Because 2-chloro-1,3-butadiene has more specific toxic effects, the QSAR approach cannot be used for this compound (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , (sub-)acute as well as (sub-)chronic toxicity data are available (part II; appendix C). All data are from one taxonomic group, namely mammals (mouse, rat, hamster). The lowest LC_{50} is 197 mg/m³ (DCV) for mice. A study with rats resulted in a NOAEL for reproduction of 0.05 mg/m³ (DCV) (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

In rats and hamsters exposure to 2-chloro-1,3-butadiene for 6 hours per day, 5 days per week for 4 weeks resulted in a slight decrease in body weight and behavioral effects in rats, and in slight irritation and restlessness in hamsters at the lowest dose of 1400 mg/m³ (DCV: 250 mg/m³) (IARC, 1979^a). In rats exposed to 200 or 1200 mg/m³ (DCV: 65 or 400 mg/m³) for 5 months, depression of the central nervous system occurred, body weight was decreased and slight blood changes were observed (Nyström, 1948).

Mutagenicity and carcinogenicity

The compound was mutagenic in *Salmonella typhimurium* and induced recessive lethal mutations in *Drosophila melanogaster*. 2-Chloro-1,3-butadiene vapour did not induce gene mutations in V79 Chinese hamster cells. It caused chromosome aberrations in-vitro in bone marrow cells and spleen lymphocytes of rats. The compound was positive in dominant lethal assays with mice and rats (Van Went & Canton, 1984; IARC, 1979^a).

No carcinogenic effects were observed in studies with rats after oral, subcutaneous or intratracheal exposures. The tumour incidence was not enhanced in mice after dermal application. The substance was classified in group 3 by IARC (IARC, 1987). From the available data the substance was considered to be genotoxic. Carcinogenicity data were inadequate (Rademaker and Van de Plassche, 1993).

Teratogenicity and reproduction

Pregnant rats were exposed from day 4 through day 16 of gestation to 0, 36, 90, 270 or 630 mg/m³ for 6 hours per day. Maternal toxicity was observed at 270 and 630 mg/m³. The NOAEL for embryotoxicity/foetotoxicity is 90 mg/m³ (DCV: 23 mg/m³) (Draper, 1991).

The evaluation of the reproductive effects is complicated by the degradation into more toxic products before use. In rats exposed continuously to 0.05, 0.15 or 1.69 mg/m³ for 4.5 months these degradation products are damaging to the testis and show foetotoxicity and embryotoxicity at concentrations of 0.15 and 1.69 mg/m³ (Sanotskii, 1976). However, male reproduction was not impaired when these male rats were exposed to pure 2-chloro-1,3-butadiene up to a concentration of 77.5 mg/m³ (DCV: 13 mg/m³), 4 hours per day for 22 days (Culik et al., 1978).

Human studies

In workers functional disturbances in spermatogenesis and morphological sperm abnormalities were observed after exposure to concentrations of impure 2-chloro-1,3-butadiene several times higher than 2 mg/m³ (Sanotskii, 1976).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

No MPC and NC in surface water can be derived because neither experimentally obtained toxicity data nor NOEC values obtained by application of QSARs are available (Van de Plassche et al., 1993).

3.2 Soil

Because neither toxicity data on organisms exposed to contaminated soil nor an MPC for aquatic organisms are available, no MPC and NC in soil can be derived (Van de Plassche and Bockting, 1993).

3.3 Sediment

Because neither toxicity data on sediment-dwelling organisms nor an MPC for aquatic organisms are available, no MPC and NC in sediment can be derived (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the NOEL value of 0.05 mg/m³, the extrapolated MPC_{eco} is determined as 5 µg/m³ (Rademaker et al., 1993).

Based on the available data, 2-chloro-1,3-butadiene cannot be excluded from being a genotoxic carcinogen, which necessitates a non-threshold approach for deriving an MPC_{human}. However, appropriate carcinogenicity data needed for low-dose risk extrapolation are not available. It was therefore decided to use the following pragmatic approach: for several other genotoxic carcinogens, MPCs, which varied from 3 to 100 µg/m³ with an accepted risk of 10⁻⁶ per year, have been derived previously (Rademaker et al., 1993). Based on this range, it is decided to set the MPC_{human} at 1.0 µg/m³ for 2-chloro-1,3-butadiene (Rademaker and Van de Plassche, 1993). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 1.0 µg/m³. The NC in air is 0.010 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	-	-	-	1.0
NC	-	-	-	0.010

4. Harmonization of MPCs and NCs

Harmonization of MPCs is not possible, because no MPCs have been derived for surface water, soil and sediment (Van de Plassche and Bockting, 1993).

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3-CHLOROPROPENE

1. Introduction

3-Chloropropene is a colourless liquid with a pungent garlic-like odour. The compound is used as an intermediate in the manufacturing of epichlorohydrin, glycerol, allyl alcohol, diallyl phthalate, fine chemicals and pharmaceuticals (IARC, 1985).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 107-05-1

Molecular formula : C_3H_5Cl

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 3-chloropropene (Van de Plassche and Bockting, et al., 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
76.53	0.118	1.45	1.4	1.4	10.0	No	38.0

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air ($10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available only on freshwater organisms: acute data on fish and amphibians; chronic data on bacteria, blue and green algae and protozoans. The NOEC values are derived from tests with insensitive species, based on a comparison of acute and chronic data (part II; appendix C). The lowest NOEC is 3.2 mg/l for green algae. The lowest LC_{50} is 0.34 mg/l for amphibians (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , only some acute and sub-chronic toxicity data are available (part II; appendix C). All data are from one taxonomic group, namely mammals. 4-Hour LC_{50} values were reported to be 1,113 mg/m³ (DCV) for both mice and rats. A NOAEL value of 27 mg/m³ (DCV) for teratogenic effects from a study with rats and rabbits is available (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

From the available subchronic toxicity studies it can be concluded that the liver, kidneys and lungs and the central nervous system are the target organs. Studies have been carried out in mice, rats, rabbits and cats with exposures varying from 5 weeks to 6 months. In rats exposed to 31, 155 or 310 mg/m³ for 8-hours per day, 5 days per week for 34 weeks neurotoxicity was observed at the two highest dose levels. The NOAEL for neurotoxicity in this study was 31 mg/m³ (DCV: 7.38 mg/m³) (Nagano et al., 1991).

Mutagenicity and carcinogenicity

3-Chloropropene is mutagenic to bacteria (*Salmonella typhimurium*) and yeast (*Saccharomyces cerevisiae*). It did not induce chromosomal aberrations in mammalian (rat liver) cells in-vitro (EPA, 1991^c; IARC, 1985).

There is inadequate evidence for the carcinogenic effects on experimental animals. In the absence of epidemiological data, no evaluation could be made of its carcinogenicity to humans. The compound was classified in group 3 by IARC (IARC, 1985).

Teratogenicity and reproduction

No embryotoxic and teratogenic effects were observed in rats and rabbits exposed to concentrations up to 930 mg/m³ (DCV: 273 mg/m³) for 7 hours per day from day 6 through day 15 and day 6 through day 18 of gestation, respectively (John et al., 1983).

Reproduction studies have not been carried out. No histopathological effects were observed on the testes after subchronic exposure of rats to concentrations varying from 9.3 to 775 mg/m³ (Torkelson et al., Quast et al., 1982^a, 1982^b).

Human studies

Motor and sensory neurotoxic damage of the distal parts of the extremities was reported in workers exposed for 2.5 months to 6 years to concentrations varying from 2.6 - 6,650 mg/m³, with a mean concentration of 2,966 mg/m³ (He et al., 1985).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because 5 chronic NOEC values were available, the method of Aldenberg and Slob could be applied to calculate the MPC. However, the distribution of NOEC values is rejected as being log-logistically distributed at a significance level of 1%. Therefore, the MPC in surface water is calculated with the modified EPA method. The MPC, using an assessment factor of 100 on the lowest LC₅₀, is 3.4 µg/l (Van de Plassche et al., 1993). The NC in surface water is 0.034 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated using the MPC for aquatic organisms by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 0.0048 mg/kg, the NC is 4.8*10⁻⁵ mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 0.0048 mg/kg and 4.8*10⁻⁵ mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀, the extrapolated MPC_{eco} is determined as 1,100 µg/m³ (Rademaker et al., 1993).

Since 3-chloropropene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. Because of the uncertainties in the human exposure data, the MPC_{human} is derived by applying an uncertain factor (UF) of 1,000 to the NOAEL of 7.38 mg/m³ (DCV), obtained from the neurotoxicity study in rats. So the MPC_{human} is 7.4 µg/m³ (Rademaker and Van de Plassche, 1993). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 7.4 µg/m³. The NC in air is 0.074 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	3.4	0.0048	0.0048	7.4
NC	0.034	$4.8 \cdot 10^{-5}$	$4.8 \cdot 10^{-5}$	0.074

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has accordingly been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentration in air is calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is only 0.07 times higher than the MPC in air, indicating that the MPC in air will not be exceeded, the MPC in surface water is not adjusted (Van de Plassche and Bockting, 1993). The MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

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1,1-DICHLOROETHANE

1. Introduction

1,1-Dichloroethane is a volatile, oily liquid. The largest individual use of 1,1-dichloroethane is as an intermediate in the manufacture of other products such as vinyl chloride, 1,1,1-trichloroethane, and to a lesser extent high vacuum rubber. It also has a limited use as a cleaning agent and a degreaser (ATSDR^a, 1990).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 75-34-3

Molecular formula : $C_2H_4Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,1-dichloroethane (Van de Plassche and Bockting, 1993)

MW	K_{ow}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
98.96	0.158	1.79	3.1	3.1	0.10	No	30.2

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Because 1,1-dichloroethane can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , acute and semi-chronic are available (part II; appendix C). All data are from one taxonomic group, namely mammals (rat, guinea pig, rabbit, cat). One LC_{50} of 23,787 mg/m^3 (DCV) for rats is available. A NOAEL of 732 mg/m^3 (DCV) for mortality was available from a semi-chronic study with rats, guinea pigs, rabbits and cats (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Subchronic studies were performed in five test animals, e.g. rats, guinea pigs, rabbits, cats and dogs. The corrected NOAELs varied from 366 mg/m^3 (on haematology and biochemistry in cats) to 854 mg/m^3 (on pathology and biochemistry in rats, guinea pigs, rabbits and dogs). NOAELs were within the same range for all species (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

The mutagenicity data are inconclusive (EPA, 1990^a).

The IARC did not classify 1,1-dichloroethane, whereas the EPA classified the compound as a possible human carcinogenic (EPA, 1990^a).

Teratogenicity and reproduction

Exposure during pregnancy resulted in a NOAEL on teratogenicity of 7,805 mg/m³ in the rat (Rademaker et al., 1993).

Although some data on reproduction are available, this information is not complete (Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

The MPC in surface water is derived using NOEC values obtained by application of QSARs. These estimated NOECs are used as input data for the method of Aldenberg and Slob. The calculated MPC in surface water is 7,300 µg/l, the NC is 73 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 23 mg/kg, the NC is 0.23 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 23 mg/kg and 0.23 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value, the extrapolated MPC_{eco} is determined as 24,000 µg/m³ (Rademaker et al., 1993).

Since 1,1-dichloroethane is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the lowest NOAEL of 366 mg/m³, so the MPC_{human} is 366 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 366 µg/m³, the NC is 3.7 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	7,300	23	23	366
NC	73	0.23	0.23	3.7

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty in the method. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived. For the time being, the MPCs and NCs for 1,1-dichloroethane for water, soil and sediment are set equal to the ones for 1,2-dichloroethane (Van de Plassche and Bockting, 1993). In table 3 an overview of the MPCs and NCs is given.

1,1-dichloroethane

Table 3: Overview of harmonised Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs)

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	700	1.5	1.5	370
NC	7.0	0.015	0.015	3.7

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1,2-DICHLOROETHANE

1. Introduction

1,2-Dichloroethane is a volatile liquid with a chloroform odour. The compound is mainly used as an intermediate in the production of vinyl chloride and in a less extent in the production of vinylidene chloride, 1,1,1-trichloroethane, trichloroethylene, aziridines and ethylene diamines (ATSDR^b, 1993). Reducing the emission of 1,2-dichloroethane to air to zero is technically impossible which means that humans and animals will always be exposed via ambient air. However, exposure must be reduced to an acceptable risk level.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 107-06-2

Molecular formula : $C_2H_4Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2-dichloroethane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
98.96	0.050	1.48	2.1	2.1	0.10	No	8.53

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Acute and chronic toxicity data are available on freshwater as well as on marine organisms (part II; appendix C). Regarding the toxicity data it seems that freshwater organisms are more sensitive than marine organisms. However, there is not enough evidence to conclude that the sensitivity of freshwater and marine organisms differ significantly. The data sets for saltwater and freshwater organisms are therefore combined to calculate the MPC in surface water (Rademaker et al., 1993). Because 1,2-dichloroethane has narcotic effects, the MPC in water is also derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , toxicity data from short-term tests and (semi-)chronic tests are available (part II; appendix C). All data are from one taxonomic group, namely mammals. The lowest LC_{50} is 265 mg/m³ (DCV) for mice, the lowest LOEL is 2 mg/m³ (DCV) for rats (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on 1,2-dichloroethane (Ministry of VROM, 1984^b).

(Sub)chronic toxicity

Semi-chronic tests (tests with an exposure time of less than 1 year) have been performed on several test species, e.g. rats, rabbits, guinea pigs, dogs and monkeys. From short-term or long-term exposure studies it can be concluded that exposures to low levels of 1,2-dichloroethane will

term exposure studies it can be concluded that exposures to low levels of 1,2-dichloroethane will particularly affect the liver and the kidneys (Heppel et al., 1946; Spreafico et al., 1980).

Repeated exposure to a concentration of 730 mg/m³ resulted in a higher mortality of rats and guinea pigs. In addition, effects on liver, kidney and growth were observed in rats, monkeys and guinea pigs (Heppel et al., 1946). Rats exposed 10 times for 6 hours per day to 607 mg/m³ within 2 weeks did not show any adverse effects (Reitz et al., 1982).

In a long-term exposure study rats are exposed to 5, 40, 202 or 607 mg/m³ for 7 hours per day and 5 days per week during a period of 2 years. Effects on liver and kidney appeared at the highest exposure concentration (Spreafico et al., 1980).

Mutagenicity and carcinogenicity

1,2-Dichloroethane is weak mutagenic in *Salmonella typhimurium* (Reitz et al., 1982; Principe et al., 1981; Van Bladeren, 1981), in *Drosophila melanogaster* (King et al., 1979; Nylander et al., 1978) and in some in-vivo and in-vitro tests using mammalian cells (Hatch et al., 1983; Storer and Conolly, 1983).

The substance was found to be carcinogenic to rats and mice after oral exposure to 47 mg per kg body weight for 78 weeks, 5 times per week (National Cancer Institute, 1978). After inhalation, fibromas and fibroma-adenomas of the mammary glands were found in female rats (Maltoni et al., 1980). Also after dermal exposure the compounds seemed to be carcinogenic (Van Duuren et al., 1979).

Teratogenicity and reproduction

A teratogenicity study was performed with female rats and rabbits. An exposure concentration of 405 mg/m³, 7 hours per day from the 6th day of pregnancy onwards resulted in effects on the rabbit dams. A concentration of 1,215 mg/m³ was toxic to the rat dam (Rao et al., 1980).

Effects on reproduction were found in a 2-generation test after exposure of rats to 57 mg/m³, 4 hours per day and 6 days per week during a period of 6 to 9 months. Effects occurred in the newborn rats (Vosovaya, 1974). In another reproduction study (Rao et al., 1980) no effects appeared on the rats after exposure to 607 mg/m³, 6 hours per day and 5 days per week during a period of 2 months.

Human studies

There are no adequate controlled studies and no recent occupational studies available (Ministry of VROM, 1984^b).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 14,000 µg/l (Van de Plassche et al., 1993). The NC in surface water is 140 µg/l (table 2).

3.2 Soil

No toxicity data are available on organisms exposed to contaminated soil. The MPC in soil is therefore calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 29 mg/kg (Van de Plassche and Bockting, 1993). The NC in soil is 0.29 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 29 mg/kg and 0.29 mg/kg respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 100 on the lowest available LOEC of 2 mg/m³, the extrapolated MPC_{eco} is determined as 20 µg/m³ (Rademaker et al., 1993).

1,2-Dichloroethane is considered as a potential genotoxic carcinogen, which necessitates a non-threshold approach for deriving an MPC_{human}. The MPC for humans is based on the 78-week study with rats and mice with an effect concentration of 47 mg/kg body weight per day (National Cancer Institute, 1978). In the calculation of the concentration corresponding to the accepted cancer risk of 10⁻⁶ per year. The assumption is made that the incidence of carcinogenicity resulting from exposure to equal doses by inhalation and by digestion is the same. The calculated MPC for humans is 48 µg/m³ (Ministry of VROM, 1984^b). Because of the uncertainties in the extrapolation formula (formula 22) the National Health Council has set the concentration at 100 µg/m³ (National Health Council, 1986^c).

Despite the fact that the MPC_{eco} is lower than the derived MPC for humans, the MPC in air is set at 100 µg/m³ (Rademaker et al., 1993) (table 2).

No NC for air is derived since the MPC for air was based on too limited data.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	14,000	29	29	100
NC	140	0.29	0.29	-

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision is made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Based on this calculation, the steady-state concentration in air is 26 times higher than the MPC in air. Therefore the MPC in surface water must be adjusted downwards. Using an adjustment factor of 20, the harmonized MPC in surface water is calculated to be 700 µg/l (table 3). Consequently the MPCs in soil and sediment are recalculated using the equilibrium partition method (Van de Plassche and Bockting, 1993). In table 3 an overview of the harmonized MPCs and NCs is given.

Table 3: Overview of harmonized Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs)

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	700	1.5	1.5	100
NC	7.0	0.015	0.015	-

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1,1-DICHLOROETHENE

1. Introduction

1,1-Dichloroethene is a volatile liquid which polymerizes readily. It is used as an intermediate for captive organic chemical synthesis and in the manufacture of polyvinylidene chloride copolymers. These polymers are used extensively in many types of flexible packing materials as flame retardant coatings and in piping coating for steel pipes and adhesive applications. The major application of the copolymers is in the production of flexible films for food packaging (ATSDR^a, 1993).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 75-35-4

Molecular formula : $C_2H_2Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,1-dichloroethene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
96.94	0.663	1.86	3.6	3.6	4.0	No	72.4

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

No toxicity data are available on freshwater or marine organisms. Because 1,1-dichloroethene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{aco} , many toxicity data are available, (sub-)acute as well as (sub-)chronic (part II; appendix C). All data are from one taxonomic group, namely mammals (mouse, rat, guinea pig, hamster, rabbit, dog, monkey). The lowest LC_{50} is 77 mg/m³ (DCV) for mice, the lowest NOAEL is 20 mg/m³ (DCV) for monkeys (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

From the available subchronic and chronic toxicity studies it can be concluded that the liver is the target organ. Groups of rats, guinea pigs, rabbits, dogs and monkeys were continuously exposed to 0, 20, 61, 101 or 189 mg/m³ for 90 days. In rhesus monkeys body weight loss, mortality and histopathological changes in the liver were observed at the two highest concentrations. At 61 mg/m³ the only effect in monkeys was a decrease in body weight. The NOAEL on growth was set at 20 mg/m³ (Rademaker and Van de Plassche, 1993; Prendergast et al., 1967).

Hepatocellular fatty changes were observed in the liver of rats exposed to 100 mg/m³ (DCV: 18 mg/m³) up to 18 months, in a 24-month toxicity and oncogenicity study. The observed changes had disappeared after 24 months (Quast et al., 1986).

Mutagenicity and carcinogenicity

1,1-Dichloroethene is mutagenic to *Salmonella typhimurium* and *Escherichia coli*. It did not cause chromosomal aberrations in mammalian cells in-vitro or in-vivo. DNA damage was observed in mammalian cells both after in-vitro and in-vivo administration (EPA, 1989; IARC, 1986^b; Short et al., 1977).

There is limited evidence for the carcinogenic effects of the compound on experimental animals. In studies with mice exposed to 0 or 220 mg/m³ for 6 hours per day, 5 days per week for 12 months, a treatment related increase in the incidence of hemangiosarcomas of the liver and kidney adenocarcinomas was observed (EPA, 1989; IARC, 1986^b; Lee et al., 1977). However according to the IARC, there is inadequate evidence for the carcinogenicity of 1,1-dichloroethene to humans (IARC, 1986^b).

Teratogenicity and reproduction

At maternal toxic doses for 7 hours per day from day 6 through day 15 or day 6 through day 18 of gestation (pregnant rats: 320 mg/m³ and pregnant rabbits: 640 mg/m³) embryotoxicity and foetotoxicity were observed, but no teratogenic effects were found (Murray et al., 1979).

In a 3-generation study in which rats received 0, 50, 100 or 200 mg/l 1,1-dichloroethene in their drinking water the reproductive capacity was not affected (Nitsche et al., 1983).

Human studies

Repeated exposure of humans to low concentrations of the compound is associated with liver and renal dysfunction.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is derived using data obtained by application of QSARs. The estimated NOECs are used as input data. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 3,400 µg/l (Van de Plassche et al., 1993). The NC in surface water is 34 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 12 mg/kg (Van de Plassche and Bockting, 1993). The NC in soil is 0.12 mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 12 mg/kg and 0.12 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. For the derivation the LC₅₀ value of 359 mg/m³ is preferred to the lowest LC₅₀ value of 77 mg/m³, because the exposure time was 22-23 hours instead of 4 hours for the LC₅₀ of 77 mg/m³. By using an assessment factor of 1,000, the extrapolated MPC_{eco} is determined as 360 µg/m³ (Rademaker et al., 1993).

Since 1,1-dichloroethene is considered not to be genotoxic carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The subchronic monkey study mentioned above was preferred for the extrapolation because, firstly, monkeys are more closely related to humans than rats and mice and secondly, the monkeys were continuously exposed to the compound instead of a few hours a day and a few days a week (Rademaker and Van de Plassche, 1993). The MPC_{human} is derived by applying an uncertainty factor (UF) of 100 to the NOAEL of 20 mg/m³ of the subchronic monkey study, so the MPC_{human} is 200 µg/m³ (Rademaker and Van de Plassche, 1993). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 200 µg/m³ (Rademaker et al., 1993). The NC in air is 2.0 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	3,400	12	12	200
NC	34	0.12	0.12	2.0

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision is made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is only 3.2 times higher than the MPC in air, the MPC in surface water is not adjusted downwards (Van de Plassche and Bockting, 1993). The MPCs and NCs presented in table 2 can be regarded as a set of harmonized values.

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1,2-DICHLOROETHENE

1. Introduction

1,2-Dichloroethene, existing in cis- and trans-isomer, is a volatile liquid. It is used primarily as a chemical intermediate in the synthesis of chlorinated solvents and compounds. It has also been used as a low-temperature extraction solvent for organic materials such as dyes, perfumes and thermoplastics (ATSDR^c, 1990).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 540-59-0

Molecular formula : $C_2H_2Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2-dichloroethene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
96.94	0.071	1.86	3.6	3.6	4.0	No	31.5

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Because 1,2-dichloroethene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche and Bockting, 1993).

Air

For the derivation of an MPC_{eco} , only one acute value is available, being an LC_{50} of 21,020 mg/m³ for mice. A NOAEL of 806 mg/m³ (DCV) for mortality and growth is found for rats, rabbits, guinea pigs and dogs (part II; appendix C) (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Subchronic studies were performed in rats, rabbits, guinea pigs and dogs. The relative potencies of the cis- and trans-isomer are not known, because the exact composition of the test substance is not generally specified. Different animals appeared to be equally sensitive to the substance. The lowest chronic value was a LOAEL of 357 mg/m³ (DCV) based on biochemistry and (histo)pathology in rats, exposed 5 days per week, 8 hours per day (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

No mutagenicity or carcinogenicity data are available (Rademaker et al., 1993).

Teratogenicity and reproduction

No teratogenicity or reproduction data are available (Rademaker et al., 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is derived using NOEC values obtained by application of QSARs. These estimated NOECs are used as input data for the method of Aldenberg and Slob. The calculated MPC in surface water is 6,100 $\mu\text{g/l}$, the NC is 61 $\mu\text{g/l}$ (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 5). The calculated MPC in soil is 22 mg/kg, the NC is 0.22 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 4). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 22 mg/kg and 0.22 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC_{50} value, the extrapolated MPC_{eco} is determined as 21,000 $\mu\text{g/m}^3$ (Rademaker et al., 1993).

The $\text{MPC}_{\text{human}}$ is derived by applying an uncertainty factor (UF) of 10,000 to the lowest LOAEL of 357 mg/m^3 , resulting in an $\text{MPC}_{\text{human}}$ of 36 $\mu\text{g/m}^3$. Since the $\text{MPC}_{\text{human}}$ is lower than the MPC_{eco} , the MPC in air is set at 36 $\mu\text{g/m}^3$ (Rademaker et al., 1993). The NC in air is 0.36 $\mu\text{g/m}^3$ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	6,100	22	22	36
NC	61	0.22	0.22	0.36

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty in the method. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived (Van de Plassche and Bockting, 1993).

DICHLOROMETHANE

1. Introduction

Dichloromethane is a clear, colourless, volatile liquid. Most applications of the compound are based on its considerable solubility and its low boiling point. The main applications are: solvent in spray cans, in paint and varnish stripper, degreaser in surface treatment (metals), extracting agent (foodstuff industry), solvent/reaction medium in the chemical/pharmaceutical industry, cleaner in the synthetics processing (polyester, polyurethane), in the production of fibres, in the surface treatment of synthetics, and solvent for lacquers and glues (Slooff and Ros, 1988).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 75-09-2

Molecular formula : $C-H_2-Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for dichloromethane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
84.93	0.039	1.25	1.8	1.8	0.14	No	46.5

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data are available on freshwater organisms as well as marine organisms (part II; appendix C). For freshwater organisms data are available on bacteria, algae, crustaceans, fish and amphibia (Van Apeldoorn et al., 1988). For marine organisms data are only available on fish. The lowest LC_{50} is 330 mg/l for marine fish (Van de Plassche et al., 1993). Since dichloromethane can be narcotic, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Slooff and Ros, 1988; Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , (sub-)chronic toxicity data are available (part II; appendix C). All data are from one taxonomic group, namely mammals (mouse, rat, gerbil, dog). The lowest NOAEL present is 124 mg/m³ (DCV) for mortality and growth for mice, calculated as LOAEL/10 (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the integrated criteria document on dichloromethane (Slooff and Ros, 1988) and the briefing report of the RIVM (RIVM, 1997).

(Sub)chronic toxicity

In animals the main target organs for dichloromethane toxicity are the liver and the central nervous system. Rats and mice continuously exposed to 347 mg/m³ during 100 days showed changes in the liver (fatty changes) and the kidneys (tubular damage) (Haun et al., 1972). In a long-term inhalation study rats were exposed to 0, 173, 694 and 1,730 mg/m³ for 6 hours per day and 5 days

dichloromethane

days per week during 20 (male) or 24 (female) months. Distinct hepatotoxicity was observed at levels > 694 mg/m³. No effects were observed at 173 mg/m³ (Nitschke et al., 1982).

Mutagenicity and carcinogenicity

Dichloromethane is mutagenic in bacteria (Simmon et al., 1977; Gocke et al., 1981). In two tests with mammalian (Chinese hamster) cells, in-vitro chromosomal aberrations were induced (Thilagar and Kumaroo, 1983; Van Apeldoorn et al., 1988). No gene mutations were detected in mammalian cells in-vitro (Jongen et al., 1981). The compound did not reveal mutagenic activity in in-vivo studies with mammals for chromosomal aberrations (Burek et al., 1984) and micronuclei (Gocke et al., 1981). A weak increase in the induction of sister chromatid exchanges (SCE) in mammalian cells in-vitro was found (Jongen et al., 1981; Thilagar and Kumaroo, 1983).

In an inhalation study mice were exposed to 0, 6,940 and 13,880 mg/m³ for 6 hours per day, 5 days per week for 102 weeks. Increased incidences of lung and liver tumours were found at both levels (NTP, 1985^b). In three carcinogenicity studies with rats increased incidences of benign mammary tumours were observed (Burek et al., 1984; Nitschke et al., 1982). Despite the high levels of exposure (up to and including 13,880 mg/m³), in none of these studies a shift from benign to malignant tumours was found. According to a recent re-evaluation by IARC (1986) and EPA (1985) there was considered to be sufficient evidence for carcinogenicity in experimental animals. Due to several uncertainties in test results however, there is not sufficient ground to consider the compound as a potential human carcinogen (Slooff and Ros, 1988).

Teratogenicity and reproduction

In fetuses of mice and rats, exposed to 4,340 mg/m³ for 7 hours per day, on day 6 through day 15 of gestation, dichloromethane induced dilated pelvis and extra sternbrae. These findings are not considered as evidence for teratogenic activity (Schwetz et al., 1975).

No reproductive impairment in rats was found in a two generation reproduction study at exposure levels of 347, 1,730 or even 5,200 mg/m³ for 6 hours per day, 5 days per week (Nitschke et al., 1985).

Human studies

The predominant effects in humans are nervous system depression and an elevated carboxyhaemoglobin level of the blood. However, no exposure-related subjective symptoms, neurobehavioural effects, motor nerve conduction velocity changes, changes in electrocardiograms, or clinical effects were reported in workers exposed to 260 to 347 mg/m³ for several years (Cherry et al., 1981). Two cases of permanent damage to the central nervous system in high long-term occupational exposures have been reported: one man exposed to levels of 2,290 to 12,500 mg/m³ for 5 years (Weiss, 1969) and another exposed to 1,735 to 3,470 mg/m³ for 3 years (Barrowcliff and Knell, 1979). The RIVM described a linear relationship between dichloromethane in the air and carboxyhaemoglobin level of the blood (RIVM, 1997).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 20,000 µg/l. The NC is 200 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 36 mg/kg, the NC is 0.36 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 36 mg/kg and 0.36 mg/kg respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value of 124 mg/m³ for mice, the extrapolated MPC_{eco} is determined as 12,000 µg/m³ (Rademaker et al., 1993).

The compound produces tumours at levels which also results in cell damage. Because the compound is not a mutagenic agent, it is considered appropriate to derive an MPC_{human} via a threshold approach.

The MPC_{human} is derived based on the assumption that there is a linear relationship between dichloromethane in the air and carboxyhaemoglobin level of the blood. Based on cut off point of 0.1% for the tolerable exceedance of carboxyhaemoglobin due to exposure to dichloromethane, an MPC_{human} of 25,000 µg/m³ for a four hour exposure can be derived (RIVM, 1997). The MPC in air is set at 25,000 µg/m³ (table 2) (RIVM, 1997). The NC in air is 20 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	20,000	36	36	25,000 ¹
NC	200	0.36	0.36	20 ²

1 Value applicable for 4 hours of exposure

2 Yearly average value

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from literature and data from the Dutch Emission Registration have been screened. The decision is made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is only 2.2 times higher than the MPC in air, the MPC in surface water is not adjusted downwards. The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values (Van de Plassche and Bockting, 1993). Because the MPC and NC in air have been adjusted only recently, no harmonisation of MPC and NC has taken place yet.

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1,2-DICHLOROPROPANE

1. Introduction

1,2-Dichloropropane is a volatile colourless liquid, which is used as an insecticidal soil fumigant. The compound is also used as an industrial solvent for oil, fats, resins, waxes and rubber, in ion exchange manufacture, in Toluene Diisocyanate production, in photographic film manufacture, for paper coating and for petroleum catalyst regeneration (ATSDR^b, 1989).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 78-87-5

Molecular formula : C₃H₆Cl₂

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,2-dichloropropane (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
112.97	0.053	1.99	2.4	2.4	0.10	No	6.0

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = Vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater and marine organisms. For freshwater organisms, acute data are available on crustaceans and fish; chronic data on fish. For marine organisms only acute data are available on algae, molluscs and fish (part II; appendix C). The lowest NOEC is 6 mg/l for freshwater fish (Van de Plassche et al., 1993).

Since 1,2-dichloropropane can have narcotic effects, the QSAR approach is used to derive the MPC in surface water (Van de Plassche et al., 1993).

Soil/sediment

On organisms exposed via contaminated soil only one value is available: an LC₅₀ of 4,240 mg/kg for oligochaeta (Van de Plassche et al., 1993).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, acute and chronic toxicity data are only available for mammals (part II; appendix C). The lowest LC₅₀ value was 952 mg/m³ (DCV) for mice. The lowest chronic value is a NOAEL of 43 mg/m³ (DCV) for growth from a study with rats (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

From subchronic toxicity studies the target organs appeared to be the nasal cavity and the blood. Studies were performed in mice, rats and rabbits with exposures for 13 weeks, 5 days per week and 6 hours per day. In rats and mice exposed to 69.3, 231 or 693 mg/m³ (DCV: 12.4, 41 and 123 mg/m³, respectively) the most critical adverse effect was degeneration of the olfactory epithelium of the nasal cavity. The NOAEL on this effect found in rats is considered to be 69.3 mg/m³ (DCV: 12.4 mg/m³) (Nitschke, 1988).

Mutagenicity and carcinogenicity

In-vitro 1,2-dichloropropane is mutagenic to bacteria (*Salmonella typhimurium*) and fungi (*Aspergillus nidulans*). In in-vivo the compound was not mutagenic to *Drosophila melanogaster* (IARC, 1986).

In mice, administered orally 125 or 250 mg/kg body weight for 103 weeks, 5 days per week, a dose-related increase of hepatocellular tumours was observed. In rats inconclusive results were obtained with females. There was no effect on the tumour incidences in male rats. For humans no data were available. The substance was classified in group 3 by IARC (IARC, 1986; 1987).

Teratogenicity and reproduction

1,2-Dichloropropane, administered to rabbits, caused foetal toxicity at a maternally toxic dose. No teratogenic effects were observed at a concentration of 150 mg/kg body weight (ATSDR^b, 1989; EPA, 1991^a).

The compound did not induce testicle degeneration, or affect sperm production up to oral dose levels of 250 mg/kg body weight (ATSDR^b, 1989).

Human studies

Acute and repeated exposure of humans to unknown concentrations caused renal failure, acute liver damage, haemolytic anemia, disturbed coagulation and respiratory irritation. These effects could be reversed after cessation of exposure. Two cases of allergic dermatitis were attributed to 1,2-dichloropropane in workers in the plastic industry (EPA, 1991^a).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC, using the method of Aldenberg and Slob is 5,300 µg/l (Van de Plassche et al., 1993). The NC in surface water is 53 µg/l (table 2).

3.2 Soil

The MPC in soil is calculated with the modified EPA method, applying an assessment factor of 1,000 on the LC₅₀ value. The MPC is 4.2 mg/kg, the NC is 0.042 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC is 13 mg/kg, the NC is 0.13 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀, the extrapolated MPC_{eco} is determined as 1,000 µg/m³ (Rademaker et al., 1993).

Since 1,2-dichloropropane is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the NOAEL of 12.4 mg/m³ (DCV), obtained from the 13-week study in rats, resulting in an MPC_{human} of 12.4 µg/m³ (Rademaker and Van de Plassche, 1993). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 12.4 µg/m³. The NC in air is 0.12 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	5,300	4.2	13	12.4
NC	53	0.042	0.13	0.12

4. Harmonization of MPCs and NCs

In order to determine the compartments of emission, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is 76 times higher than the MPC in air, the MPC in surface water must be adjusted downwards. Using an adjustment factor of 70, the harmonized MPC in surface water is calculated to be $76 \mu\text{g/l}$. The NC is $0.76 \mu\text{g/l}$ (table 3). Consequently, the MPC and NC in sediment are recalculated using the equilibrium partitioning method (Van de Plassche and Bockting, 1993). In table 3 an overview of the harmonized MPCs and NCs is given.

Table 3: Overview of harmonized Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs)

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	76	4.2	0.18	12
NC	0.76	0.042	$1.8 \cdot 10^{-3}$	0.12

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1,3-DICHLOROPROPANE

1. Introduction

The compound 1,3-dichloropropane is a volatile liquid. Since information about its use is not available, it is not possible to indicate where it is presently used and which products contain this compound.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 142-28-9

Molecular formula : $C_3H_6Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,3-dichloropropane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
112.97	0.076	2.00	5.0	5.0	0.10	No	6.0

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only one toxicity value is available, being an LC_{50} of 87 mg/l on marine organisms (fish) (part II; appendix C). Because 1,3-dichloropropane can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , only one value is available, being an LC_{50} of 6,000 mg/m³ (DCV) for the rat (part II; appendix C) (Rademaker et al., 1993).

2.3 (Human) toxicity data

No useful (human) toxicity data are available.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is derived using NOEC values obtained by application of QSARs. These estimated NOECs are used as input data of the method of Aldenberg and Slob. The calculated MPC in surface water is 5,200 µg/l, the NC is 52 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 26 mg/kg, the NC is 0.26 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 26 mg/kg and 0.26 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the LC_{50} value, the extrapolated MPC_{eco} is determined as $6,000 \mu\text{g}/\text{m}^3$ (Rademaker et al., 1993).

Since no (human) toxicity data are available at all, no MPC_{human} could be derived (Rademaker and Van de Plassche, 1993). Thus the MPC in air is set equal to the MPC_{eco} , being $6,000 \mu\text{g}/\text{m}^3$. The NC in air is $60 \mu\text{g}/\text{m}^3$ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs), and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	5,200	26	26	6,000
NC	52	0.26	0.26	60

4. Harmonization of MPCs and NCs

The harmonization procedure is not carried out for 1,3-dichloropropane, since only effect-data are available to calculate an MPC in air, aiming at the protection of the ecosystem and not at the protection of human beings. When more (human) toxicity information becomes available, a new MPC in air can be derived. For the time being, the MPCs and NCs for 1,3-dichloropropane in water, soil and sediment are set equal to the ones for 1,2-dichloropropane because the harmonization procedure is carried out for 1,2-dichloropropane and in addition the toxicity of 1,3-dichloropropane is comparable to the toxicity of 1,2-dichloropropane (Van de Plassche and Bockting, 1993). In table 3 an overview of these values is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs)

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	76	0.18	0.18	6,000
NC	0.76	$1.8 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$	60

1,3-DICHLOROPROPENE

1. Introduction

1,3-Dichloropropene, existing as a cis- and trans-isomer, is a chloroform-like, light-coloured liquid with a sharp, sweet, penetrating and irritating odour. It is used in agriculture as soil fumigant for parasitic nematodes (IARC, 1986).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 542-75-6
Molecular formula : $C_3H_4Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,3-dichloropropene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
110.97	0.029	1.76	2.9	2.9	12.6	No	4.5

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and for sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data are available on freshwater organisms (crustaceans and fish) and marine organisms (algae, crustaceans and fish) (part II; appendix C). The lowest LC_{50} is 0.8 mg/l for marine crustaceans (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , many (sub-)acute as well as (sub-)chronic toxicity data are available (part II; appendix C). All data are from one taxonomic group, namely mammals. The lowest LC_{50} value is 450 mg/m³ (DCV) for the rat. The lowest NOAEL value is 8 mg/m³ (DCV) for growth for rats and mice (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Subchronic and chronic toxicity studies indicate that the target organs are the urinary bladder, the uteri and the nasal cavity. In several longterm studies mice and rats were exposed to concentrations from 21 mg/m³ up to 272 mg/m³ for 5 days per week, 6 hours per day for 2 years (DCV: 4 and 49 mg/m³, respectively). Histopathological effects were observed and an increase in the incidence of benign lung tumors (Dow Chemical, 1987^a; 1987^b; Lomax et al., 1989). The NOAEL for histopathological changes in the urinary bladder and the nasal cavity, found in mice, was considered to be 21 mg/m³ (DCV: 4 mg/m³) (Lomax et al., 1989).

Mutagenicity and carcinogenicity

Both the cis- and the trans-isomer of 1,3-dichloropropene were mutagenic to bacteria. Chromosomal aberrations were observed in-vitro in cultured hamster-ovary cells. In *Drosophila melanogaster* sex-linked recessive lethal mutations were induced. In in-vivo, a micronucleus test in mice and a host-mediated assay were negative (IARC, 1986; ACT, 1993).

For animals, evidence on carcinogenicity was available, based on oral tests in mice and rats (NTP, 1985^a; IARC, 1986). From recent studies in rats and mice 1,3-dichloropropene was concluded not to be carcinogenic via the inhalatory route. No increase in malignant tumours was observed at any concentration during exposure for 2 years (Dow Chemical, 1987^a; 1987^b; Lomax et al., 1989; Stott et al., 1988). For humans inadequate data were available. The substance was classified in group 2B by IARC (IARC, 1986; 1987).

Teratogenicity and reproduction

No teratogenic effects were observed in rats and rabbits exposed to 91, 272 or 545 mg/m³ from day 6 through day 15 or day 5 through day 18 of gestation, respectively. In rats embryotoxic effects were observed at maternal toxic doses. In rabbits maternal toxicity was observed at the two highest concentrations, but no embryotoxicity was seen (WHO, 1990^b; ACT, 1993).

No effects were observed on reproductive parameters in a 2-generation study in rats. The rats were exposed for 6 hours per day, 5 days per week, up to a concentration of 409 mg/m³ (DCV: 73 mg/m³) (ACT, 1993).

Human studies

Two cases of malignant histiocytic lymphoma were reported in firemen previously treated for acute symptoms after exposure to 1,3-dichloropropene. Accidental exposure caused headache, chest discomfort and malaise. Two years after exposure these effects were still reported in 50% of the exposed people. In workers exposed to 4.5 mg/m³ 1,3-dichloropropene (TWA), sperm counts and percentages of normal sperm were normal (IARC, 1986).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated with the modified EPA method. The MPC, using an assessment factor of 100 on the lowest LC₅₀, is 8.0 µg/l (Van de Plassche et al., 1993). The NC is 0.080 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 0.023 mg/kg, the NC is 2.3*10⁻⁴ mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 0.023 mg/kg and 2.3*10⁻⁴ mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀, the extrapolated MPC_{eco} is determined as 450 µg/m³ (Rademaker et al., 1993).

Since 1,3-dichloropropene is considered to be non-carcinogenic after inhalatory exposure, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 100 to the NOAEL of 4 mg/m³ (DCV), obtained from the 2-year mouse study, resulting in an MPC_{human} of 40 µg/m³ (Rademaker and Van de Plassche, 1993). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 40 µg/m³. The NC in air is 0.40 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	8.0	0.023	0.023	40
NC	0.080	$2.3 \cdot 10^{-4}$	$2.3 \cdot 10^{-4}$	0.40

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission in surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission in water. Because the steady-state concentration in air is lower than the MPC in air, the MPC in surface water is not adjusted downwards (Van de Plassche and Bockting, 1993). The MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

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2,3-DICHLOROPROPENE

1. Introduction

2,3-Dichloropropene is a volatile liquid. Since no information about its use is available, it is not possible to say where it is presently used and what products contain it.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 78-88-6

Molecular formula : $C_3H_4Cl_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 2,3-dichloropropene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
110.97	0.052	2.04	5.5	5.5	10	No	7.1

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

No toxicity data are available on organisms exposed via contaminated surface water. Because the compound does not have any narcotic effects, the QSAR approach cannot be used (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , only an LC_{50} value of 378 mg/m³ (DCV) for rats is available (part II; appendix C) (Rademaker et al., 1993).

2.3 (Human) toxicity data

No useful (human) toxicity data are available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because no toxicity data are available, the MPC and NC in surface water are set equal to the values calculated for 1,3-dichloropropene. The MPC and NC are 8.0 µg/l and 0.080 µg/l, respectively (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 0.044 mg/kg, the NC is $4.4 \cdot 10^{-4}$ mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 0.044 mg/kg and $4.4 \cdot 10^{-4}$ mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the LC_{50} value, the extrapolated MPC_{eco} is determined as $380 \mu\text{g}/\text{m}^3$ (Rademaker and Van de Plassche, 1993).

Since not enough (human) toxicity data are available, no MPC_{human} could be derived. The MPC in air is set at the MPC_{eco} of $380 \mu\text{g}/\text{m}^3$ (Rademaker and Van de Plassche, 1993). The NC in air is $3.8 \mu\text{g}/\text{m}^3$ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	8.0	0.044	0.044	380
NC	0.080	$4.4 \cdot 10^{-4}$	$4.4 \cdot 10^{-4}$	3.8

4. Harmonization of MPCs and NCs

The harmonization procedure is not carried out for 2,3-dichloropropene, since only effect-data are available to calculate an MPC in air, aiming at the protection of the ecosystem and not at the protection of human beings. When more (human) toxicity information becomes available, a new MPC in air can be derived (Van de Plassche and Bockting, 1993).

ETHYLENE

1. Introduction

Ethylene is a colourless gas. It is produced by a variety of anthropogenic sources (petrochemical complexes) as well as natural sources (plants and micro-organisms). As a biological role, it regulates the process of growth and development and is known as an ageing hormone. It is used for the production of polyethylene, ethylene oxide, ethylene dichloride and ethyl benzene (Slooff et al., 1991°).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 74-85-1
Molecular formula : C₂-H₄

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for ethylene (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
28.05	3.072	1.13	0.67	0.67	8.50	Yes	4,040

MW = molecular weight (in g/mol)
K_{aw} = air-water partition coefficient
K_{ow} = octanol-water partition coefficient
Kp = partition coefficient (in l/kg)
k_{deg} = degradation rate constant in air (in 10⁻⁶/s)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

No reliable toxicity data are available on freshwater or marine organisms. Since ethylene is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, only one acute LC₅₀ was present for mammals while many acute as well as chronic toxicity data are available for plants. Since the experiments were not designed to establish no-observed-effect-levels, most data are presented as effect levels only. Acute data varied from 12 to 4,600 mg/m³, chronic (> 10 days) effect levels ranged from 8 to 2,300 mg/m³ (part III; appendix C) (Van der Eerden, 1987; Slooff et al., 1991°; Rademaker et al., 1993).

2.3 (Human) toxicity data

For ethylene no useful (human) toxicity data are available.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 8,500 µg/l. The NC is 85 µg/l (table 2). (Van de Plassche et al., 1993).

ethylene

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 5.8 mg/kg, the NC is 0.058 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 5.8 mg/kg and 0.058 mg/kg respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air is derived by application of the method of Aldenberg and Slob. Based on ecotoxicity data for plants, an MPC_{eco} of $2 \mu\text{g}/\text{m}^3$ (24-hour average) is calculated (Slooff et al., 1991; Rademaker et al., 1993).

No MPC_{human} can be calculated due to lack of useful data. Considering the biological role of ethylene, the MPC_{eco} is used as the NC in air. The existing limit value (determined by Van der Eerden, 1987) is $300 \mu\text{g}/\text{m}^3$ (Van de Plassche and Bockting, 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	8,500	5.8	5.8	-
NC	85	0.058	0.058	2

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision is made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche et al., 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the limit value for air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is only 4.8 times higher than the limit value for air, the MPC in surface water is not adjusted downwards. The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values (Van de Plassche and Bockting, 1993).

ETHYLENE OXIDE

1. Introduction

Ethylene oxide is a volatile liquid. It is used as an intermediate for the production of various chemicals. The compound is also used as a fumigant, a sterilant for food and cosmetics and in hospital sterilization (WHO, 1985^b).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 75-21-8

Molecular formula : C_2H_4O

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for ethylene oxide (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
44.05	12.66	-0.30	0.025	0.025	0.06	No	146

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data are available on freshwater organisms (crustaceans and fish) and marine organisms (crustaceans) (part III; appendix C). The lowest LC_{50} value is 84 mg/l for fish (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , acute as well as chronic toxicity data are available (part III; appendix C). All data are from one taxonomic group, namely mammals (mouse, rat, guinea pig, rabbit, dog, rhesus monkey). The lowest NOAEL present is 1.9 mg/m³ (DCV) for reproduction for rhesus monkeys, calculated as LOAEL/10. The lowest LC_{50} is 250 mg/m³ (DCV) for mice (Rademaker et al., 1993).

2.3 (Human) toxicity data

The following (human) toxicity data are based on the Criteria Document on ethylene oxide (Ministry of VROM, 1986^a).

(Sub)chronic toxicity

Male and female rats, exposed to 17.8, 59.0 and 182 mg/m³ ethylene oxide for a period of 25 months, 5 days per week, 6 hours per day, showed increased mortality and a decrease in body weight at the two highest concentrations. Histopathological changes were observed at the highest dose (Ministry of VROM, 1986^a).

Mutagenicity and carcinogenicity

Ethylene oxide is mutagenic to plants, microorganisms, insects, mammalian cells in-vitro as well as mammals in-vivo. The compound induces gene mutations in all studied plants, bacteria, insects and mammalian cells in-vitro as well as chromosome aberrations in plants, insects and mammalian cells in-vitro and in-vivo (Ministry of VROM, 1986^a).

In male and female rats, exposed to 17.8, 59.0 and 182 mg/m³ for a period of 25 months, 5 days per week, 6 hours per day, treatment-related leukemia and primary brain tumours were induced at the two highest concentrations. In addition, male rats developed peritoneal mesothelioma and subcutaneous fibromas (Lynch et al., 1984; Ministry of VROM, 1986^a).

Teratogenicity and reproduction

In rats and mice embryotoxicity and foetotoxicity have been observed (Laborde et al., 1980; Hackett et al., 1982). Clear teratogenic effects have been found in mice after oral administration at the highest dose of 150 mg per kg body weight (LaBorde and Kimmel, 1980), but not after inhalation by rats and rabbits (Hackett et al., 1982).

No effects on reproduction have been observed after exposure of male and female rats to 18, 58, and 173 mg/m³ ethylene oxide, 6 hours per day, 5 days per week, during a period of 12 weeks (Ministry of VROM, 1986^a).

Human studies

Occupational and/or accidental exposure causes irritation of the eyes and the respiratory system and effects on the nervous system. These reactions usually only appear after some time (Wolfs et al., 1983). Endotracheal intubation with canulas that have been sterilized with ethylene oxide, can result in serious respiratory problems, caused by infection and reversible paralysis of the vocal chords (Holley and Gildae, 1971). Repeated exposure to ethylene oxide vapour in a concentration higher than 1,000 mg/m³ can result in even more serious, but reversible effects on the nervous system. The effect on the somatic nervous system is characterized by functional disorders in the limbs (Gross et al., 1979). Residues of ethylene oxide on sterilized materials can cause haemolysis of blood in vitro (Clarke et al., 1966; Lebrech et al., 1977).

Occupational exposure to the compound in concentrations of 0.6 mg/m³ (8 hours TWA) and higher induces chromosome aberrations in lymphocytes and bone marrow cells (Stolley, 1984). In concentrations less than 1 mg/m³ an increased incidence of spontaneous abortions is observed (Hemminki et al., 1983; Yakubova et al., 1976). On the basis of mortality studies it cannot be excluded that ethylene oxide induces tumours in humans (Hogstedt et al., 1984).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated with the modified EPA method and based on acute toxicity data for freshwater and marine organisms. The MPC, using an assessment factor of 1,000 on the lowest LC₅₀, is 84 µg/l (Van de Plassche et al., 1993). The NC in surface water is 0.84 µg/l (table 2).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 0.0021 mg/kg (Van de Plassche and Bockting, 1993). The NC in soil is 2.1 * 10⁻⁵ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 0.0021 mg/kg and 2.1 * 10⁻⁵ mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value, the extrapolated MPC_{eco} is determined as 190 µg/m³ (Rademaker et al., 1993).

Based on the available data, ethylene oxide cannot be excluded from being a genotoxic carcinogen, which necessitates a non-threshold approach for deriving an MPC_{human}. The MPC derived to protect humans is based on a 25-month rat carcinogenicity study with an effect concentration of 17.8 mg/m³ (Lynch et al., 1984). The calculated MPC_{human} is 2.4 µg/m³ (Ministry of VROM, 1986^a). Because of its strong genotoxic effect, the National Health Council has set the concentration at 3 µg/m³ (National Health Council, 1992). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 3.0 µg/m³ (table 2). No NC for air is derived since the MPC for air was based on too limited data.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and negligible concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	84	0.0021	0.0021	3.0
NC	0.84	2.1*10 ⁻⁵	2.1*10 ⁻⁵	-

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is only 6 times higher than the MPC in air, the MPC in surface water is not adjusted downwards (Van de Plassche and Bockting, 1993). The MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

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HEXACHLOROETHANE

1. Introduction

Hexachloroethane is a volatile liquid. It is used as a component in fumigating candles and smoke bombs and as a degasification agent in smelted light metal (GDCh, 1989^o). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 67-72-1

Molecular formula : C_2Cl_6

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for hexachloroethane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
236.72	0.255	4.14	200	200	0.05	No	0.028

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data are available on marine organisms (part III; appendix C). The single present LC_{50} is 2.4 mg/l for fish (Van de Plassche et al., 1993).

Since hexachloroethane can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , sub-acute and sub-chronic toxicity data are available for mammals, while for birds a chronic study is available (part III; appendix C). The lowest NOAEL is 27 mg/m³ for mortality for rats, guinea pigs and dogs (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Subchronic studies were performed on rats, guinea pigs and dogs, exposed 5 days per week and 6 hours per day during 6 weeks, resulting in a NOAEL of 150 mg/m³ (DCV: 27 mg/m³), on mortality, growth and (histo)pathology. No variation in sensitivity was observed in these species (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

Mutagenicity or carcinogenicity data are not presented (Rademaker et al., 1993).

Teratogenicity and reproduction

A teratogenicity study in rats exposed from day 6 through day 16 of gestation resulted in a NOAEL on teratogenicity of 2,500 mg/m³ (DCV: 456 mg/m³) (Rademaker et al., 1993).

Reproduction data are not available (Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using method of the Aldenberg and Slob is 83 $\mu\text{g/l}$, the NC is 0.83 $\mu\text{g/l}$ (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 17 mg/kg, the NC is 0.17 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. The MPC is therefore calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 17 mg/kg and 0.17 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value for mammals, the extrapolated MPC_{eco} is determined as 2,700 $\mu\text{g/m}^3$ (Rademaker et al., 1993).

The $\text{MPC}_{\text{human}}$ is derived by applying an uncertainty factor (UF) of 1,000 to the NOAEL of 27 mg/m³ of the subchronic mammal study, resulting in an $\text{MPC}_{\text{human}}$ of 27 $\mu\text{g/m}^3$. Since the $\text{MPC}_{\text{human}}$ is lower than the MPC_{eco} , the MPC in air is set at 27 $\mu\text{g/m}^3$ (Rademaker et al., 1993). The NC in air is 0.27 $\mu\text{g/m}^3$ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	83	17	17	27
NC	0.83	0.17	0.17	0.27

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty in the MPC in air. When more toxicity information becomes available (resulting over a lower uncertainty factor to be applied) a new MPC in air can be derived (Van de Plassche and Bockting, 1993).

PENTACHLOROETHANE

1. Introduction

Pentachloroethane is a volatile liquid. It may occur as an intermediate in the production of chlorinated ethylenes. The compound can be used as a solvent for cellulose plastics, natural gums and resins and for dry-cleaning, as a drying agent for timber and for coal purification (IARC, 1986). For the derivation of harmonized MPCs and NCs the bioaccumulation potential has not yet been studied.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 76-01-7

Molecular formula : C_2HCl_5

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for pentachloroethane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
202.28	0.036	3.63	210	210	0.05	No	0.453

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are only available on marine organisms (part III; appendix C). The only present LC_{50} is 116 mg/l for fish. The lowest NOEC is 10 mg/l for algae (Van de Plassche et al., 1993).

Since pentachloroethane is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , no useful data are available (Rademaker et al., 1993).

2.3 (Human) toxicity data

For the derivation of an MPC_{human} , no useful (human) toxicity data are available (Rademaker et al., 1993; Rademaker and Van de Plassche 1993).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 230 $\mu g/l$, the NC is 2.3 $\mu g/l$ (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 49 mg/kg, the NC is 0.49 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 49 mg/kg and 0.49 mg/kg respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	230	49	49	-
NC	2.3	0.49	0.49	-

4. Harmonization of MPCs and NCs

The harmonization procedure is not carried out for pentachloroethane, since no MPC in air is available. Therefore, the MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

1,1,2,2-TETRACHLOROETHANE

1. Introduction

1,1,2,2-Tetrachloroethane is a volatile liquid. It is used in the production of trichloroethylenes, tetrachloroethylenes and 1,2-dichloroethylene. Due to the toxicity of the compound and new processes for manufacturing chlorinated ethylenes, the use of 1,1,2,2-tetrachloroethane now appears to be very limited (ATSDR^c, 1989).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 79-34-5

Molecular formula : C₂H₂Cl₄

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,1,2,2-tetrachloroethane (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
167.85	0.014	2.39	4.2	4.2	0.10	No	0.793

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are only available on marine organisms (part III; appendix C). The only present value is an LC₅₀ of 12 mg/l for fish (Van de Plassche et al., 1993).

Since 1,1,2,2-tetrachloroethane is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, only acute data for mammals (mice and rats) are available. The lowest LC₅₀ is 583 mg/m³ (DCV) for rats (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

Two subchronic studies were performed in rats and rabbits and resulted in NOAELs varying from 2 to 10 mg/m³ (DCV: 0.2 to 1 mg/m³). The sensitivity of both species were comparable.

In both studies the animals were exposed for only 3-4 hours per day, resulting in a lowest NOAEL of 0.2 mg/m³ (DCV) based on hematology and biochemistry (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

Mutagenicity data are not presented (Rademaker et al., 1993).

Limited evidence on carcinogenicity is available for animals. For humans the evidence available is inadequate. The compound was classified by IARC in group 3 (IARC, 1979^b; 1987).

Teratogenicity and reproduction

Teratogenicity studies and useful reproduction data are not presented (Rademaker et al., 1993; Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker et al., 1993).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because in general toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob is 3,300 $\mu\text{g/l}$, the NC is 33 $\mu\text{g/l}$ (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 14 mg/kg, the NC is 0.14 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 14 mg/kg and 0.14 mg/kg respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC_{50} value for rats, the extrapolated MPC_{eco} is determined as 583 $\mu\text{g/m}^3$ (Rademaker et al., 1993).

The $\text{MPC}_{\text{human}}$ is derived by applying an uncertainty factor (UF) of 1,000 to the NOAEL of 0.20 mg/m³ of the subchronic studies, resulting in an $\text{MPC}_{\text{human}}$ of 0.20 $\mu\text{g/m}^3$. Since the $\text{MPC}_{\text{human}}$ is lower than the MPC_{eco} , the MPC in air is set at 0.20 $\mu\text{g/m}^3$ (Rademaker et al., 1993). The NC in air is 0.0020 $\mu\text{g/m}^3$ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	3,300	14	14	0.20
NC	33	0.14	0.14	0.0020

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as a coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty in the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived (table 2) (Van de Plassche and Bockting, 1993).

TETRACHLOROETHENE

1. Introduction

Tetrachloroethene (PER) is a volatile colourless liquid, which is used primarily as a solvent in dry-cleaning industry. Other major industrial uses of the compound includes the cleaning and degreasing of metals and the production of chlorofluorocarbons (CEPA, 1993^o). It is also used in metal degreasing (Ministry of VROM, 1984^o). For the derivation of harmonized MPCs and NCs the bioaccumulation potential of the compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS number : 127-18-4

Molecular formula : C_2Cl_4

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for tetrachloroethene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
165.82	0.364	3.40	12	12	0.17	No	1.87

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in pKa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms (part III; appendix C). For freshwater organisms acute and chronic data are available on crustaceans and fish. For marine organisms, only acute data are available on molluscs and fish. The lowest NOEC is 0.51 mg/l for crustaceans (Van de Plassche et al., 1993).

Since tetrachloroethene can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

For tetrachloroethene one LC_{50} of 155 mg/kg soil is available on oligochaeta (part III; appendix C) (Van de Plassche et al., 1993).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , only for mammals (mouse, rat, gerbil) are data available (part III; appendix C). The lowest LC_{50} is 5,050 mg/m³ (DCV) for mice. The lowest NOAEL is 12.3 mg/m³ (DCV) for mortality in mice, calculated as LOAEL/10 (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on tetrachloroethene (Ministry of VROM, 1984^o) and the briefing report of the RIVM (RIVM, 1996).

(Sub)chronic toxicity

Subchronic studies were performed in rats, mice, rabbits guinea pigs and monkeys. The most important target organs are the liver, central nervous system and the kidneys. Rats exposed for 8 weeks, 4 hours per day, 5 days per week to 1,356 mg/m³ showed fatty infiltration in the liver and an increase in extractable fat, but no cirrhosis or necrosis (Kylin et al., 1965).

Mutagenicity and carcinogenicity

Tetrachloroethene is not mutagenic to *Escherichia coli* (Greim et al., 1975). In bone-marrow cells of mice and rats, no chromosomal aberrations were induced after single, repeated, or long-term exposure in vivo (Cherna and Kypernova, 1977). In host-mediated assays with *Salmonella typhimurium* strains and female ICR mice as hosts, an increase in mutagenic effects was observed. No dose-dependency was found (Cherna and Kypernova, 1977).

No clear differences in the incidence of different tumour types were observed in an inhalation study in which rats were exposed to 2,100 and 4,010 mg/m³ for 6 hours per day, 5 days per week, during 12 months (Rampy et al., 1978). Evidence from epidemiological studies among dry cleaning and laundry workers is insufficient to conclude that exposure to tetrachloroethene can cause cancer in humans (Blair et al., 1979; Katz and Jowett, 1981). The WHO concluded that there was not enough evidence to consider tetrachloroethene as carcinogen and for this reason based the guideline value within the framework of the Air Quality Guidelines (AQG) on a study with non-neoplastic effects (WHO, 1995).

Teratogenicity and reproduction

Rats exposed to 2,060 mg/m³ on day 6 through day 15 of pregnancy showed reduced body weight and a slightly increased number of resorptions (Schwetz et al., 1975). No teratogenic effects were found. In the same study, pups of mice, exposed to 2,060 mg/m³ on day 6 through day 15 of pregnancy showed a reduced body weight, delayed ossification of skull bones, an increase in the incidence of subcutaneous oedema and split sternbrae.

Tetrachloroethene did not cause any reproductive toxicity when rats and rabbits were exposed to 3,390 mg/m³ during pregnancy (Hardin et al., 1981).

Human studies

In an occupational-exposure study dry-cleaning workers were exposed from 678 to 2,712 mg/m³. They showed signs of central nervous system depression and in many cases the autonomic nervous system was also affected. Liver malfunction was not observed (Münzer and Heder, 1972). In another study, subjects exposed for 1, 3 or 7.5 hours per day, for 5 days per week, did not show any effects at 136 mg/m³. At 678 and 1,017 mg/m³, coordination was slightly impaired (Hake and Steward, 1977). The WHO based their guidelines value (AQG), i.e. 250 µg/m³, on a LOAEL of 102 mg/m³ from a study with dry-cleaning workers showing starting kidney damage (WHO, 1995). The ATSDR derived a NOAEL of 272 µg/m³ from an epidemiological study with persons exposed to tetrachloroethene for a period of about 10 years (mean concentration 15 ppm) (ATSDR, 1995).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 330 µg/l, the NC is 3.3 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

The MPC in soil is calculated using the modified EPA method and applying an assessment factor of 1,000 on the LC₅₀ value. The MPC is 0.16 mg/kg, the NC is 0.0016 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). The MPC in sediment is 4.0 mg/kg. The NC is 0.040 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value for mice, the extrapolated MPC_{eco} is 1,200 µg/m³ (Rademaker et al., 1993).

Since tetrachloroethene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by the RIVM in their briefing report (RIVM, 1996^b). Starting point for the derivation were two epidemiological studies used by the WHO and ATSDR to derive a minimal risk limit. The MPC_{human} is 250 µg/m³ (RIVM, 1996^b). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 250 µg/m³ (RIVM, 1996^b). The NC in air is 2.5 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	330	0.16	4.0	250
NC	3.3	0.0016	0.040	2.5

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from literature and data from the Dutch Emission Registration have been screened. The decision is made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is lower than the MPC in air, the MPC in surface water is not adjusted downwards (Van de Plassche and Bockting, 1993). The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values. Because the MPC and NC in air have been adjusted only recently, no harmonisation of MPC and NC has taken place yet.

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TETRACHLOROMETHANE

1. Introduction

Tetrachloromethane is a volatile colourless liquid, which is used primarily for the production of those chlorofluorocarbons that act primarily as refrigerants (ATSDR^a, 1989).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 56-23-5

Molecular formula : C-Cl₄

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for tetrachloromethane (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	K _{deg}	Readily biodegradable	Vp
153.82	0.637	2.83	34	34	0.05	No	11.9

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

K_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and for sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data are available on marine organisms (fish) (part III; appendix C) (Van de Plassche et al., 1993).

Since tetrachloromethane can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, only for mammals (mouse, rat, guinea pig) data are available (part III; appendix C). The lowest LC₅₀ is 11,525 mg/m³ (DCV) for female mice. The lowest NOAEL is 6.1 mg/m³ (DCV) for mortality for rats and guinea pigs (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the criteria document on tetrachloromethane (Ministry of VROM, 1986^b).

(Sub)chronic toxicity

In all toxicity studies performed, the main target organs appeared to be the liver and the kidneys. In a 90-day study rats, guinea pigs, rabbits, dogs and monkeys were continuously exposed to a concentration of 0, 6.1 or 61 mg/m³. The exposure to 61 mg/m³ resulted in growth retardations and histopathological changes in the liver in all animals exposed. At 6.1 mg/m³ only a slight reduction of growth was seen in the rats (Prendergast et al., 1967).

Mutagenicity and carcinogenicity

In several studies tetrachloromethane appeared not to be mutagenic to bacteria (*Escherichia coli*, *Salmonella typhimurium*) (Barber et al., 1981; Cooper and Witmer, 1982; De Flora, 1981). Two limited host-mediated assays with *Salmonella typhimurium* strains and mice, were both negative (Braun and Schoneich, 1975; Shapiro and Fonshtein, 1979). Studies of DNA damage were performed in bacteria and in mammalian cells in vitro and yielded some positive (De Flora et al., 1984) as well as negative results (Perocco and Prodi, 1981). The results of most of the in vivo studies for DNA damage in liver cells of mice and rats were negative (Mirsalis et al., 1982).

Repeated administration of tetrachloromethane leads to the formation of hepatomas in a number of animal species. In mice, induction of hepatomas was found at dose levels of 256, followed by 380 mg/kg body weight (Andervont, 1958) and at 1,250 and 2,500 mg/kg body weight (NCI, 1976^a; 1976^b). In rats induction of hepatomas was found at a dose level of 2080 mg/kg body weight (Reuber and Glover, 1970). There is evidence that tetrachloromethane-treatment via several routes of administration can induce liver tumours in both sexes of several animal species when repeated hepatonecrotic doses are used. The compound has a tumour-promoting activity (Ministry of VROM, 1986^b).

There is no evidence to relate the occurrence of cancer in humans to exposure to tetrachloromethane (EPA, 1984^a).

Teratogenicity and reproduction

Pregnant female rats were exposed to 0, 2,140 or 6,430 mg/m³ for 7 hours per day, during day 6 through day 15 of gestation. Food consumption in the dams was decreased and signs of hepatotoxicity were observed at both dose levels. No effects on litter size and live fetuses/litter were observed. In both exposure groups fetuses with skeletal variations were found (Schwetz et al., 1974^b).

No adequate study exists on the effects of tetrachloromethane on animal reproduction. Only studies at fairly high dose levels (1,500 and 2,370 mg/kg body weight) have been performed (Kalla and Bansal, 1975).

Human studies

In man, as in animals, the liver is the main target organ of tetrachloromethane toxicity. Exposure leads to severe liver damage (jaundice) and renal disfunction.

However, in most studies reliable data on dose levels are lacking, or exposure to tetrachloromethane goes together with exposure to other chemicals or interfering factors (Ministry of VROM, 1986^b).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 1,100 µg/l, the NC is 11 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated using the MPC for aquatic organisms by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 37 mg/kg. The NC is 0.37 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 37 mg/kg and 0.37 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value for rats and guinea pigs, the extrapolated MPC_{eco} is 610 µg/m³ (Rademaker et al., 1993).

The compound produces liver tumours at exposure levels which also result in cell damage. Because the compound is not a mutagenic agent, it is considered appropriate to derive an MPC_{human} via a threshold approach. The MPC_{human} is derived by applying an uncertainty factor of 100 to the NOAEL for rats and guinea pigs of 6.1 mg/m³ (DCV) on the liver and kidneys, obtained from the 90-day study resulting in an MPC_{human} of 60 µg/m³ (Ministry of VROM, 1984; Rademaker et al., 1993). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 60 µg/m³ (table 2) (Rademaker et al., 1993). No NC for air is derived since the MPC for air was based on too limited data.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	1,100	37	37	60
NC	11	0.37	0.37	-

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision is made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is only 3.9 times higher than the MPC in air, the MPC in surface water is not adjusted downwards. The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values (Van de Plassche and Bockting, 1993).

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1,1,1-TRICHLOROETHANE

1. Introduction

1,1,1-Trichloroethane is a volatile colourless liquid which is used as a solvent for metal cleaning and degreasing and as a solvent in various formulations, including adhesives, paints, inks, dry-cleaning agents and typewriter correction fluids. The compound is also extensively used in household products (ATSDR^d, 1990).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 71-55-6

Molecular formula : $C_2H_3Cl_3$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,1,1-trichloroethane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
133.41	0.415	2.49	3.3	3.3	0.01	No	13.3

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms (part III; appendix C). For freshwater organisms acute data are available on green algae, bacteria, crustaceans and fish and chronic data also on blue algae. For marine organisms only acute data are available on fish. The lowest NOEC is 1.3 mg/l for crustaceans (Van de Plassche et al., 1993).

Since 1,1,1-trichloroethane is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , data are available for plants and mammals (part III; appendix C). For mammals (mouse, rat, rabbit, gerbil, guinea pig, dog and rhesus monkey) only chronic and subchronic data are available: the lowest NOAEL being 145 mg/m³ (DCV) for growth for rats in a 2-year study. For plants the lowest LC₅₀ is 19,000 mg/m³ (DCV) for growth (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

From several studies the target organs appeared to be the liver and the brain (Rademaker and Van de Plassche, 1993). In two 3-month studies gerbils were exposed to 0, 380, 1,134 or 5,400 mg/m³. In different brain areas, DNA concentrations were significantly decreased and effects were observed on the astroglial cell population in the cerebral cortex at the two highest concentrations (Rosengren et al., 1985; Karlsson et al., 1987). In another study, rats and mice were exposed to 0, 810, 2,700 or 8,100 mg/m³ (DCV: 145, 482 and 1,446 mg/m³) for 24 months, 5 days per week, 6 hours per day. In the highest exposure group of rats body weights were decreased and very slight hepatic effects were observed. The NOAEL for rats in this study was 2,700 mg/m³ (DCV: 482 mg/m³) (Quast et al., 1988).

Mutagenicity and carcinogenicity

1,1,1-Trichloroethane is not mutagenic to bacteria. In-vitro assays with mammalian cells were negative, except for a chromosomal aberration test in Chinese hamster cells without metabolic activation. The compound was negative in the available in-vivo mammalian tests. A host-mediated assay was also negative (WHO, 1992^a; EPA, 1990^b).

From inhalation and oral studies, performed in mice and rats, inadequate evidence on carcinogenicity is available (Quast et al., 1988; IARC, 1979). For humans no data are available. 1,1,1-trichloroethane is classified by IARC in group 3 (IARC, 1979; 1987)

Teratogenicity and reproduction

Mice and rats were exposed to 4,700 mg/m³, 7 hours per day during gestation from day 6 through day 15. No teratogenic effects were observed (Schwetz et al., 1975^b).

In a 2-generation study with mice, no effects were observed on reproduction parameters up to an oral dose of 1,000 mg/kg body weight (Lane et al., 1982). In male rats exposed for 6 months to 2,700 mg/m³ (DCV: 563 mg/m³), no histopathological effects were observed on the testes (Torkelson et al., 1958).

Human studies

Acute inhalatory exposure of humans caused mild eye irritation, nervous system effects, cardiac arrhythmia, mild liver effects, unconsciousness and decreased blood pressure. The effects of long-term exposure are not known (ATSDR, 1990^d; WHO, 1992^a).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because in general more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 2,100 µg/l, the NC is 21 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 6.9 mg/kg, the NC is 0.069 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 6.9 mg/kg and 0.069 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value for rats, the extrapolated MPC_{eco} is rounded off to 15,000 µg/m³ (Rademaker et al., 1993).

Since 1,1,1-trichloroethane is considered to be non-carcinogenic after inhalatory exposure, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor (UF) of 100 to the NOAEL of 482 mg/m³ (DCV), obtained from the 2-year rat study, resulting in an MPC_{human} of 4,820 µg/m³. Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 4,800 µg/m³ (Rademaker and Van de Plassche, 1993). The NC in air is 48 µg/m³ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	2,100	6.9	6.9	4,800
NC	21	0.069	0.069	48

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentration in air is calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is lower than the MPC in air, the MPC in surface water is not adjusted downwards (Van de Plassche and Bockting, 1993). The MPCs and NCs presented in table 2 can be regarded as a harmonized set of values.

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1,1,2-TRICHLOROETHANE

1. Introduction

1,1,2-Trichloroethane is a volatile liquid. The principal use of the compound is as a chemical intermediate in the production of 1,1-dichloroethene. It has also minor uses: as a solvent for the coating laid down on films and as a chemical intermediate or process solvent in pharmaceutical manufacture (IARC, 1979).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 79-00-5

Molecular formula : $C_2H_3Cl_3$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for 1,1,2-trichloroethane (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
133.39	0.017	1.89	4.9	4.9	0.33	No	3.0

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms (part III; appendix C). For freshwater organisms acute data are available on green algae, molluscs, crustaceans and fish and chronic data also on bacteria and blue algae. For marine organisms acute data are available on algae, annelides, crustaceans, molluscs and fish and chronic data on annelides, crustaceans and fish. The lowest NOEC is 3.0 mg/l for marine fish (Van de Plassche et al., 1993).

Since 1,1,2-trichloroethane can have narcotic effects, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , only acute data for mammals (mice and rats) are available. The lowest LC_{50} is 397 mg/m³ (DCV) for rats (Rademaker et al., 1993).

2.3 (Human) toxicity data

(Sub)chronic toxicity

No chronic or subchronic inhalation studies are available. Several subchronic and chronic oral studies are present. Tested species, rats and mice, were equally sensitive. The lowest NOAEL of 3.9 mg/kg body weight based on biochemistry, growth and hematology, was obtained from a 90-day study in mice. Converting this NOAEL value to continuous inhalation exposure results in a NOAEL of 18.2 mg/m³ (Rademaker et al., 1993).

Mutagenicity and carcinogenicity

For 1,1,2-trichloroethane mutagenicity or carcinogenicity data are not presented (Rademaker et al., 1993).

Teratogenicity and reproduction

Teratogenicity or reproduction toxicity data are not available (Rademaker et al., 1993; Rademaker and Van de Plassche, 1993).

Human studies

Human studies are not available (Rademaker and Van de Plassche, 1993).

3. Derivation of MPCs and NCs for different compartments**3.1 Surface water**

Because in general more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 7,900 $\mu\text{g/l}$, the NC is 79 $\mu\text{g/l}$ (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 39 mg/kg, the NC is 0.39 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 39 mg/kg and 0.39 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC_{50} value for rats, the extrapolated MPC_{eco} is rounded off to 400 $\mu\text{g/m}^3$ (Rademaker et al., 1993).

The MPC_{human} is derived by applying an uncertainty factor (UF) of 1,000 to the NOAEL of 18.2 mg/m³ (converted to inhalation exposure) of the oral subchronic study, resulting in an MPC_{human} of 18.2 $\mu\text{g/m}^3$. Since the MPC_{human} is lower than the MPC_{eco} , the MPC in air is set at 18 $\mu\text{g/m}^3$ (Rademaker et al., 1993). The NC in air is 0.18 $\mu\text{g/m}^3$ (table 2).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	7,900	39	39	18
NC	79	0.39	0.39	0.18

4. Harmonization of MPCs and NCs

Based on the harmonization procedure of the MPCs in water, soil and sediment with the one in air, the MPCs cannot be considered as coherent set of values. Since the MPC in air is based on the modified EPA method (preliminary effect assessment method), the MPC in surface water is not adjusted because of the uncertainty in the MPC in air. When more toxicity information becomes available (resulting in a lower uncertainty factor to be applied) a new MPC in air can be derived (Van de Plassche and Bockting, 1993).

TRICHLOROETHENE

1. Introduction

Trichloroethene is a volatile colourless liquid, which is mainly used for the vapour degreasing and cold cleaning of fabricated metal parts. It has also been used as a solvent formulator in plastic-processing, glues, cleaners and stain removers (Ministry of VROM, 1984^d; WHO, 1985^a).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 79-01-6

Molecular formula : C_2HCl_3

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for trichloroethene (Van de Plassche and Bockting, 1993)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
131.39	0.149	2.42	5.5	5.5	2.36	No	7.71

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993)

2.2 Ecotoxicity data

Surface water

Many toxicity data are available on freshwater as well as marine organisms (part III; appendix C). For freshwater organisms acute data are present on bacteria, crustaceans, insects, coelenterates, molluscs, fish and amphibians. Chronic data are available on bacteria, blue and green algae, protozoans and fish. For marine organisms acute data are available on algae, annelides, crustaceans, molluscs and fish and chronic data on annelides. The lowest NOEC is 5.8 mg/l for freshwater fish (Van de Plassche et al., 1993).

Because trichloroethene can have narcotic effects, the MPC for surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco} , only for rats and mice data are available (part III; appendix C). The lowest LC_{50} is 7,567 mg/m³ (DCV) for mice. Only one NOAEL of 189 mg/m³ (DCV) for growth for rats is available (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on trichloroethene (Ministry of VROM, 1984^d).

(Sub)chronic toxicity

Trichloroethene toxicity is related mainly to central nervous system depression. In a 90-day study rats, guinea pigs, rabbits, dogs and monkeys were continuously exposed to trichloroethene in a concentration of 189 mg/m³. The only observed effect was on growth of all species except dogs (Prendergast et al., 1967).

Mutagenicity and carcinogenicity

In studies with pure trichloroethene negative results (Barbin et al., 1978; Waskell, 1978) and weakly positive results (Crebelli et al., 1982; Greim et al., 1975; 1977; Longstaff, 1980) in bacteria (*Escherichia coli*, *Salmonella typhimurium*) after metabolic activation were reported. In yeast negative and positive results were also found. In several other mutagenicity studies, in-vitro as well as in-vivo, conflicting results were found. In-vitro DNA-binding studies showed strong binding capacity after metabolic activation only (Miller and Guengerich, 1983). In-vivo studies revealed only very weak binding to DNA (Bergman, 1983).

In an inhalation study mice and rats were exposed 6 hours per day, 5 days per week during 18 months to 0, 540, 1,620 and 3,250 mg/m³ trichloroethene. Only in mice were significantly increased incidences of hepatocellular carcinoma seen (Audit of Ind. Bio-Test Lab., 1979). Several other studies with mice, rats and hamsters did not show any increased tumour incidences. From the available epidemiological studies no evidence of a positive correlation between exposure to trichloroethene and cancer in man could be detected (Axelson et al., 1978).

Teratogenicity and reproduction

Despite a doubtful result in one rabbit study (Beliles et al., 1980^b; Hardin et al., 1981), no teratogenic properties of trichloroethene could be demonstrated, only embryotoxic effects such as retarded ossification were seen in the following studies: one study with pregnant mice exposed to 1,620 mg/m³ (DCV: 473 mg/m³) 7 hours per day during day 6 through day 15 of pregnancy (Schwetz et al., 1975^b) and another study with rats exposed before and/or during pregnancy to 2,700 mg/m³ (DCV: 675) 6 hours per day (Beliles et al., 1980^b; Hardin et al., 1981). Reproduction studies are not available (Ministry of VROM, 1984^d).

Human studies

For man the narcotic and neurotoxic properties of trichloroethene represent the main health hazard. In workers exposed up to 20 years to concentrations ≤ 540 mg/m³ no changes in EEG or psychometric field tests were reported, nor any haematological changes or changes in hepatic function (Boudène et al., 1983). In another long-term occupational study, no effects on the central nervous system were observed in workers exposed chronically to 270 mg/m³ (Triebig et al., 1977).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 2,400 µg/l, the NC is 24 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 13 mg/kg, the NC is 0.13 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p in sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 13 mg/kg and 0.13 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 1,000 on the lowest LC₅₀ value for mice, the extrapolated MPC_{eco} is 7,600 µg/m³ (Rademaker et al., 1993).

Since trichloroethene is considered to be non-carcinogenic, a threshold approach for deriving an MPC_{human} is justified. The MPC_{human} is derived by applying an uncertainty factor of 100 to the NOAEL of 189 mg/m³ (DCV), obtained from the 90-day study with mammals, so the MPC_{human} is 1,900 µg/m³ (Ministry of VROM, 1984^d).

trichloroethene

However, the Dutch National Health Council advised use of the NOAEL obtained from the human occupational study performed by Triebig et al. (1977). Using an uncertainty factor of 13, they derived an MPC_{human} of 5 mg/m³ (National Health Council, 1985). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 5,000 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	2,400	13	13	5,000
NC	24	0.13	0.13	50

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is lower than the MPC for air, the MPC for surface water is not adjusted downwards. The MPCs and NCs presented in table 2 can therefore be regarded as a harmonized set of values (Van de Plassche and Bockting, 1993).

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TRICHLOROMETHANE

1. Introduction

Trichloromethane (chloroform) is a volatile colourless liquid. Most of the trichloromethane production is used for the production of chlorodifluoromethane. This latter product is used mainly in cooling installations and for the preparation of fluorohydrocarbon polymers (Ministry of VROM, 1986^d).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 67-66-3
Molecular formula : C-H-Cl₃

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for trichloromethane (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
119.38	0.074	1.97	3.2	3.2	0.10	No	21.3

MW = molecular weight (in g/mol)
K_{aw} = air-water partition coefficient
K_{ow} = octanol-water partition coefficient
Kp = partition coefficient (in l/kg)
k_{deg} = degradation rate constant in air (in 10⁻⁶/s)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater as well as marine organisms (part III; appendix C). As for freshwater organisms acute data exist for green algae, crustaceans and fish. Chronic data are available on bacteria, blue and green algae and crustaceans. For marine organisms chronic data are only available on algae. The lowest LC₅₀ is 18 mg/l for fish and the lowest NOEC is 9.7 mg/l for marine crustaceans (Van de Plassche et al., 1993).

Because trichloromethane is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, data are available only for mammals (mouse, rat, dog) (part III; appendix C). The lowest NOAEL is 4.3 mg/m³ (DCV) for reproduction in rats, calculated as LOAEL/10 (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on chloroform (Ministry of VROM, 1986^d).

(Sub)chronic toxicity

In a 6-month study, rats were exposed to trichloromethane in concentrations of 0, 110, 230 and 410 mg/m³ for 7 hours per day and 5 days per week. In both male and female rats, renal and hepatic damage were observed. No effects were seen in the male rats after 1, 2 or 4 hours exposures to the 110 mg/m³ level using the same schedule of exposure (Torkelson et al., 1976).

Mutagenicity and carcinogenicity

Trichloromethane has been tested in a variety of mutagenicity and indicator tests. A few positive results were observed, amongst others, in non-mammalian eukaryotic systems, e.g. yeasts (Callen et al., 1980; Loprieno, 1981) and in in-vivo mammalian testing, e.g. micronucleus tests in mice (Agustin and Lim-Sylianco, 1978). These results, however, require further experimental support, and, as yet, they do not justify the consideration of trichloromethane as a mutagenic agent (Ministry of VROM, 1986^d).

In a study with mice, the compound was administered in corn oil by gavage 5 times a week for 78 weeks in dose levels of 0, 138, 238, 277 and 477 mg/kg body weight, a dose related increase in the formation of hepatocellular carcinomas was observed. In the same study, in rats given trichloromethane at the same schedule in dose levels of 0, 90 and 180 mg/kg body weight, dose-related increased frequencies of kidney epithelial tumours were observed (NCI, 1976^a). In another study with mice, the compound was administered in toothpaste by gavage, 6 days a week for a 80-weeks period at dose levels of 0, 17 and 60 mg/kg body weight per day. Kidney tumours were formed in the high dose group (Roe et al., 1979). A causal relation between trichloromethane in drinking water and cancer in man is very unclear (Wilkins et al., 1979).

Teratogenicity and reproduction

In a study with pregnant rats, exposed to concentrations of 0, 146, 490 and 1460 mg/m³ for 7 hours per day during day 6 through day 15 of gestation, embryo and fetotoxicity (resulting in reduced pregnancy and increased resorption) were found at 146 mg/m³ (DCV: 43 mg/m³). Minor skeletal aberrations (retarded ossification) were reported at all levels. No teratogenic effects were reported (Schwetz et al., 1974^a).

In a three-generation study with mice, effects on fertility were only observed at the highest dose level of 1000 mg/kg body weight per day, a dose level which caused severe hepatotoxicity and death, too (Borzelleca and Carchman, 1982).

Human studies

Occupational exposure to trichloromethane in the range of either 80 to 160 mg/m³ for less than 4 months (Phoon et al., 1983) or 10 to 1000 mg/m³ for 1 to 4 years (Bomski et al., 1967) caused liver toxicity (toxic jaundice).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Because more toxicity data are available using the QSAR approach than can be obtained from the literature, the MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 5,900 µg/l, the NC is 59 µg/l (table 2) (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 19 mg/kg, the NC is 0.19 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p in sediment is equal to the K_p in soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 19 mg/kg and 0.19 mg/kg, respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value for rats, the extrapolated MPC_{eco} is 430 µg/m³ (Rademaker et al., 1993).

The compound produces tumours in livers and/or kidneys at levels which also result in cell damage. Because the compound is not a mutagenic agent, it is considered appropriate to derive an MPC_{human} via a threshold approach. The MPC_{human} is derived by applying an uncertainty factor of 1,000 to the NOAEL of 110 mg/m³, obtained from the 6-month study with rats. This value is not amended for continuous exposure (Ministry of VROM, 1986^d). So the MPC_{human} is 100 µg/m³ (Ministry of VROM, 1986^d; Rademaker et al., 1993). Since the MPC_{human} is lower than the MPC_{eco}, the MPC in air is set at 100 µg/m³, the NC is 1.0 µg/m³ (table 2) (Rademaker et al., 1993).

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	5,900	19	19	100
NC	59	0.19	0.19	1.0

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is 11 times higher than the MPC in air, the MPCs in surface water is adjusted downwards by a factor 10. The harmonized MPCs and NCs are presented in table 3 (Van de Plassche and Bockting, 1993).

Table 3: Overview of harmonized Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs)

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	590	1.9	1.9	100
NC	5.9	0.019	0.019	1.0

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VINYLCHLORIDE

1. Introduction

Vinylchloride is a colourless vapour. It is used for the production of polyvinyl chloride and mixed polymerisates. The only other known direct application of the compound is its transformation to 1,1,2-trichloroethane which serves as the initial product for the production of 1,1-dichloroethene (GDCh, 1989^b; Ministry of VROM, 1984^a).

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 75-01-4

Molecular formula : C₂H₃Cl

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for vinylchloride (Van de Plassche and Bockting, 1993)

MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
62.50	0.646	1.52	1.7	1.7	6.60	No	33.7

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in 10⁻⁶/s)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche and Bockting, 1993).

2.2 Ecotoxicity data

Surface water

No toxicity data are available at all on freshwater or marine organisms. Since vinylchloride is acting by narcosis, the MPC in surface water is derived using the QSAR approach (Van de Plassche et al., 1993).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche et al., 1993).

Air

For the derivation of an MPC_{eco}, (sub-)acute as well as (sub-)chronic toxicity data are available (file II; appendix C). All data are from one taxonomic group, namely mammals (mouse, rat, guinea pig, rabbit). The lowest LC₅₀ is 24,479 mg/m³ (DCV) for mice. A study with rats resulted in a NOAEL for reproduction of 6 mg/m³ (DCV) (Rademaker et al., 1993).

2.3 (Human) toxicity data

The (human) toxicity data are derived from the Criteria Document on vinylchloride (Ministry of VROM, 1984^a).

(Sub)chronic toxicity

In a one-year time-sequence inhalation study rats were exposed to 13,000 mg/m³ vinylchloride for 7 hours per day, 5 days per week for 52 weeks. They generally showed a slightly shorter blood clotting time, an increased weight of heart, kidneys and spleen, and histopathological changes in liver, kidneys, heart and spleen (Feron et al., 1979). In another study, rats exposed to concentrations of 130, 1,300 or 52,000 mg/m³ for 5 hours per day, 5 days per week during 10 months showed toxic effects including morphological liver injuries at the 130 mg/m³ level (Sokal et al., 1980).

Mutagenicity and carcinogenicity

Vinylchloride vapour is mutagenic after metabolic activation in bacterial tests (*Salmonella typhimurium*) (Bartsch and Montesano, 1975), in yeast (Loprieno et al., 1976^b) and in mammalian cells in-vitro inducing gene mutations (Drevon and Kuroki, 1979). The compound caused chromosomal abnormalities in-vivo after inhalation by Chinese hamster (Basler and Röhrbron, 1980) and by rat (Del Marco et al., 1976). Mutational events in germ cells of male rat (Short et al., 1977) and mouse (Himeno et al., 1983), as measured by the dominant lethal test, are not observed. The compound is mutagenic in the Tradescantia plant assay system (Van 't Hoff and Schnairer, 1982).

In several studies vinylchloride has been found to be carcinogenic in rats when administered orally or by inhalation, and in mice, hamsters and rabbits following inhalation exposure. A dose-response effect has been demonstrated. The main types of tumours are neoplastic nodules, carcinomas and angiosarcomas of the liver, extrahepatic angiosarcomas, zymbal gland carcinomas, neuroblastomas of the brain, nephroblastomas, mammary gland carcinomas and nasal carcinomas. In rats exposed 4 hours per day, 5 days per week during 52 weeks, the two lowest concentrations to give an increase of tumours (angiosarcomas, nephroblastomas and zymbal gland tumours) were 26 and 65 mg/m³ (Maltoni et al., 1981). Vinylchloride is also carcinogenic to mice and hamsters (both exposed for 4 hours per day, 5 days per week for 30 weeks to 130 to 2,600 mg/m³ (Maltoni et al., 1981)) and rabbits (exposed for 4 hours per day, 5 days per week for 12 months to 26,000 mg/m³ (Caputo et al., 1974)). Inhalation at high concentrations in occupational exposures is carcinogenic to humans. In particular, angiosarcoma of the liver and brain cancer appeared to have increased (Dannaher et al., 1981).

Teratogenicity and reproduction

Mice, rats and rabbits were exposed to 1,300 mg/m³ for 7 hours on day 6 through day 15 (mice and rats) or day 6 through day 18 (rabbits) of gestation. Subsequently, additional groups of mice were exposed in the same way to 130 mg/m³, and rats and rabbits to 6,500 mg/m³. No embryotoxic or teratogenic effects were observed (John et al., 1977).

Human studies

After long-term occupational exposures toxic effects occurred to several organs. Neurological symptoms were reported after exposure to 130 mg/m³ and possibly to concentrations below 26 mg/m³ (Spirtas et al., 1975). Acro-osteolysis occurred in a worker exposed to 3.9-146 mg/m³ during a 2 to 5 years period (Stewart et al., 1975). Exposure to about 5.2 mg/m³ for at least 6 months gave an increased diastolic blood pressure (Hasegawa et al., 1979). Exposure to 26-260 mg/m³ gave restrictive lung disorders (Mapp et al., 1978). Liver fibrosis and other organ disorders were found after exposure for more than 100 months to at least 130 mg/m³ (Blendis et al., 1978). Several cohort studies showed a correlation between cancer incidence (especially angiosarcoma of the liver and to a lesser extent brain cancer) and occupational exposure (Waxweiler et al., 1976; Dannaher et al., 1981).

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC is derived using NOEC values obtained by application of QSARs. The calculated MPC in surface water, using the method of Aldenberg and Slob, is 8,200 µg/l. The NC is 82 µg/l (table 2). (Van de Plassche et al., 1993).

3.2 Soil

Because no toxicity data are available on organisms exposed to contaminated soil, the MPC in soil is calculated by application of the equilibrium partitioning method (formula 7). The calculated MPC in soil is 14 mg/kg, the NC is 0.14 mg/kg (table 2) (Van de Plassche and Bockting, 1993).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Because the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil, being 14 mg/kg and 0.14 mg/kg respectively (table 2) (Van de Plassche and Bockting, 1993).

3.4 Air

The MPC in air based on ecotoxicity data is derived by application of the modified EPA method. By using an assessment factor of 10 on the lowest NOAEL value for rats, the extrapolated MPC_{eco} is 600 µg/m³ (Rademaker et al., 1993).

Vinylchloride is considered to be a potential human carcinogen for which there is no threshold level. The exposure concentration corresponding to the accepted cancer risk of 10⁻⁶ per year, used for the extrapolation to humans is 26 mg/m³ (Maltoni, 1981). The calculated MPC_{human} is 35 µg/m³ (Ministry of VROM, 1984^e). This concentration is based on several assumptions and uncertainties (e.g. only one animal experiment). For this reason it is decided to set the MPC_{human} in air at 100 µg/m³ (National Health Council, 1986^a) (table 2). No NC for air is derived since the MPC for air was based on too limited data.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	8,200	14	14	100
NC	82	0.14	0.14	-

4. Harmonization of MPCs and NCs

In order to determine the emission compartments, information from the literature and data from the Dutch Emission Registration have been screened. The decision has been made to carry out the harmonization procedure for two possible situations, i.e. emission to air and emission to water (Van de Plassche and Bockting, 1993).

When emitted to air, the equilibrium concentrations do not exceed the MPCs in other compartments. Emission to surface water results in an equilibrium concentration in air higher than the MPC in air. Consequently the steady-state concentrations are calculated (using the SimpleBox model), assuming emission to water. Because the steady-state concentration in air is 14 times higher than the MPC in air, the MPC in surface water is adjusted downwards by a factor 10. Consequently the MPC and NC in soil and sediment are lowered by a factor 10. The harmonized MPCs and NCs are presented in table 3 (Van de Plassche and Bockting, 1993).

Table 3: Overview of harmonized Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs)

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	820	1.4	1.4	100
NC	8.2	0.014	0.014	-

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APPENDIX D

PESTICIDES

- ALDRIN AND DIELDRIN
- CARBOFURAN
- CHLORDANE
- CHLORPYRIFOS
- DDD
- DDE
- DDT
- ENDOSULFAN
- ENDRIN
- FENTHION
- α -HCH
- β -HCH
- HEPTACHLOR AND HEPTACHLOR EPOXIDE
- LINDANE
- QUINTOZENE
- TBTO
- THIRAM

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ALDRIN AND DIELDRIN

1. Introduction

Aldrin and dieldrin are organic substances, which were formerly used as insecticides. In the Netherlands their use has been prohibited.

Aldrin is rapidly converted to dieldrin in surface water, soil and mammals (WHO, 1989^b; Metcalf et al., 1973). A considerable amount of chronic data for dieldrin is available for aquatic organisms, birds and mammals. For this reason, all MPCs for aldrin are derived based on the data for dieldrin (except for the MPC in sediment). Consequently, only toxicity data for dieldrin are discussed in this report, while the data for aldrin and dieldrin are presented in the appendix of part III.

Both compounds have the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. aldrin : 309-00-2

Molecular formula aldrin : $C_{12}H_8Cl_6$

CAS no. dieldrin : 60-37-1

Molecular formula dieldrin : $C_{12}H_8Cl_6O$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for aldrin and dieldrin (Van de Plassche, 1994)

Substance	MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
Aldrin	364.93	-	6.50	6457	6457	-	-	-
Dieldrin	381	-	6.20	37154	37154	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Many chronic toxicity data for dieldrin are available on freshwater organisms (blue algae, molluscs, crustaceans and fish) and marine organisms, while no acute data are available (part III; appendix D). Fish seem to be especially sensitive. Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity. The lowest NOEC value is $0.12 \mu g/l$ (Van de Plassche, 1994).

Soil/sediment

Acute and chronic toxicity data are available on organisms exposed via contaminated soil: acute data for collembola; chronic data for microbial processes, insects and collembola (part III; appendix D). The lowest NOEC value is 0.5 mg/kg for collembola (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Many chronic toxicity data are available for mammals as well as for birds (part III; appendix D). Birds and mammals seem to be equally sensitive to dieldrin. The lowest NOEC is 0.5 mg/kg food (Van de Plassche, 1994).

The geometric mean whole body BCF for freshwater and marine water fish is 6,700 l/kg (with a maximum BCF of 13,000 l/kg). The calculated BCF for dieldrin (formula 10) is 76,000 l/kg. The BCF for freshwater and marine water bivalves is 2,200 l/kg (based on field data) (with a maximum BCF of 3,100 l/kg), while the calculated BCF is 21,000 l/kg (formula 11). For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

Since six chronic studies are available for dieldrin, the method of Aldenberg and Slob can be used to derive an MPC in surface water based on direct effects. This MPC, based on the combined data set for marine and freshwater organisms, is 0.029 $\mu\text{g/l}$ (Van de Plassche, 1994).

Indirect effects

Combining data sets for birds and mammals and applying the method of Aldenberg and Slob leads in the case of dieldrin to a NEC of 0.38 mg/kg food (Van de Plassche, 1994).

To calculate the MPCs for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 0.018 $\mu\text{g/l}$ (Van de Plassche, 1994).

Final MPC

Since the MPC for secondary poisoning using the BCF of fish is lower than the MPC in water based on direct effects, it can be concluded that secondary poisoning via the aquatic route may be critical. So, the final MPC for the aquatic environment is set at 0.018 $\mu\text{g/l}$ (Van de Plassche, 1994). The final NC in surface water is $1.8 \cdot 10^{-4} \mu\text{g/l}$ (table 2).

3.2 Soil

Direct effects

The MPC in soil based on direct effects of 0.050 mg/kg in standard soil is calculated using the modified EPA method applying a factor of 10 on the lowest NOEC (Van de Meent et al., 1990; Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals and calculated with the method of Aldenberg and Slob (using the BCF for earthworms) is 0.087 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is slightly higher than the MPC in soil based on direct effects. It is therefore concluded that the MPC value of 0.050 mg/kg does not need to be adjusted downwards. Thus, the final MPC in soil is set at 0.050 mg/kg, the MPC being based on direct effects on terrestrial organisms (Van de Plassche, 1994). The NC in soil is $5.0 \cdot 10^{-4} \text{ mg/kg}$ (table 2).

3.3 Sediment

For aldrin and dieldrin no toxicity data are available on sediment-dwelling organisms. The MPCs are therefore calculated using the equilibrium partitioning method (formula 6) and equal 0.12 mg/kg and 0.67 mg/kg, respectively (Van de Plassche, 1994). The NCs in sediment are 0.0012 mg/kg and 0.0067 mg/kg, respectively (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.018 (aldrin and dieldrin)	0.050 (aldrin and dieldrin)	0.12 (aldrin) 0.67 (dieldrin)	-
NC	$1.8 \cdot 10^{-4}$ (aldrin and dieldrin)	$5.0 \cdot 10^{-4}$ (aldrin and dieldrin)	0.0012 (aldrin) 0.0067 (dieldrin)	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPCs calculated by equilibrium partitioning (i.e. 0.12 for aldrin and 0.67 mg/kg for dieldrin) are both higher than the MPC in soil, based on toxicity data, being 0.05 mg/kg . In particular the value of 0.67 mg/kg (for dieldrin) is too high, being almost equal to the lowest LC_{50} . It is therefore decided that the harmonized MPC in soil should be set equal to the one based on direct effects on soil organisms, i.e. 0.05 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 21 $\mu\text{g/m}^3$ and 10 $\mu\text{g/l}$, respectively (aldrin) and 0.13 $\mu\text{g/m}^3$ and 0.40 $\mu\text{g/l}$, respectively (dieldrin) (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.018 (aldrin and dieldrin)	0.050 (aldrin and dieldrin)	0.12 (aldrin) 0.67 (dieldrin)	-
NC	$1.8 \cdot 10^{-4}$ (aldrin and dieldrin)	$5.0 \cdot 10^{-4}$ (aldrin and dieldrin)	0.0012 (aldrin) 0.0067 (dieldrin)	-
CritConc	-	-	-	21 (aldrin, air) 0.13 (dieldrin, air) 10 ¹⁾ (aldrin, rainwater) 0.40 ¹⁾ (dieldrin, rainwater)

1) The unit of the CritConc in rainwater is $\mu\text{g/l}$

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CARBOFURAN

1. Introduction

Carbofuran is an organic substance which is used as an insecticide, acaricide and nematocide. The compound has a cholinesterase-inhibiting effect. Carbofuran might have the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS number : 1563-66-2
Molecular formula : $C_{12}H_{15}N-O_3$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for carbofuran (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
221.28	-	2.32	2.14	2.14	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 K_p = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater and marine organisms. For freshwater organisms, acute data are available on insects, fish and amphibia and chronic data on crustaceans and fish. For marine organisms, acute and chronic data are available on crustaceans and fish (part III; appendix D). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity to carbofuran. The lowest NOEC available is $0.5 \mu g/l$ for saltwater crustaceans. The lowest LC_{50} value is $1.5 \mu g/l$ (Van de Plassche, 1994).

Soil/sediment

Chronic as well as acute toxicity data are available for soil organisms: acute data for nematods, oligochaetes, collembola and insects; chronic data for bacteria, fungi and oligochaetes (part III; appendix D). The lowest NOEC is $0.5 mg/kg$ for oligochaetes and the lowest LC_{50} $0.47 mg/kg$ for collembola (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Birds may be slightly more sensitive to carbofuran than mammals, although only three NOECs are available for each group (part III; appendix D). The lowest NOEC for birds is $2.6 mg/kg$ food and for mammals $17 mg/kg$ food (Van de Plassche, 1994).

No reliable experimental BCFs were found. A value of $2.6 l/kg$ is presented in a limited test. This value supports indications found in literature that carbofuran has no bioaccumulating potency. The calculated BCF for fish (formula 10) is $10 l/kg$, and the one for bivalves (formula 11) is $3 l/kg$. For earthworms a mean BCF of $1 l/kg$ (with a maximum BCF of $10 l/kg$) is assumed (Van de Plassche, 1994).

carbofuran

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

Even though no toxicity data are available for algae, the modified EPA method is used to derive the MPC based on direct effects, applying a factor of 100 instead of 1,000 on the lowest LC₅₀. This is considered acceptable because a considerable amount of NOECs and LC₅₀s are available for fish, amphibia, crustaceans and insects. The MPC based on the combined data sets for marine and freshwater organisms is 0.015 µg/l (Van de Plassche, 1994).

Indirect effects

The MPC, based on the combined data sets for birds and mammals and calculated with the method of Aldenberg and Slob, is 2.0 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data sets of birds and mammals, is 64 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is much higher than the MPC in water based on direct effects. This is caused by the low BCF. It is therefore concluded that there will probably be no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC for the aquatic environment is set at 0.015 µg/l (Van de Plassche, 1994). The NC in surface water is $1.5 \cdot 10^{-4}$ µg/l (table 2).

3.2 Soil

Direct effects

Even though no toxicity data are available for plants or arthropodes, the modified EPA method is used to derive an MPC in soil, applying a factor of 100 instead of 1,000 on the lowest LC₅₀. This is considered acceptable because acute data are present for at least four taxonomic groups. The MPC in soil is 0.0047 mg/kg in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals and calculated with the method of Aldenberg and Slob (using the BCF for earthworms) is 0.46 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is much higher than the MPC in soil based on direct effects, indicating that there will probably be no risk of secondary poisoning via the terrestrial route. Thus, the final MPC in soil is set at the one based on direct effects on terrestrial organisms, i.e. 0.0047 mg/kg (Van de Plassche, 1994). The NC in soil is $4.7 \cdot 10^{-5}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore an MPC of $3.2 \cdot 10^{-5}$ mg/kg is calculated using the equilibrium partitioning method (formula 6) (Van de Plassche, 1994). The NC in sediment is $3.2 \cdot 10^{-7}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.015	0.0047	$3.2 \cdot 10^{-5}$	-
NC	$1.5 \cdot 10^{-4}$	$4.7 \cdot 10^{-5}$	$3.2 \cdot 10^{-7}$	-

4. Harmonization of MPCs and NCs

Because only MPCs for surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. $3.2 \cdot 10^{-5} \text{ mg/kg}$) is circa 150 times lower than the MPC based on toxicity data, being 0.0047 mg/kg (table 2). Several factors may be responsible for this large difference, e.g. the uncertainty in the relatively low K_p of 2.14 l/kg , or characteristics of tests with soil organisms. On the one hand it can be argued that concentrations in pore water above the MPC for aquatic organisms may cause adverse effects. On the other hand, terrestrial toxicity data are available for target organisms. It is decided to set the harmonized MPC in soil at 0.0047 mg/kg (value), the MPC based on direct effects on soil organisms (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $0.0005 \mu\text{g/m}^3$ and $2 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.015	0.0047	$3.2 \cdot 10^{-5}$	-
NC	$1.5 \cdot 10^{-4}$	$4.7 \cdot 10^{-5}$	$3.2 \cdot 10^{-7}$	-
CritConc				0.0005 (air) 2 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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CHLORDANE

1. Introduction

Chlordane is an organic substance, which was formerly used as an insecticide. In the Netherlands its use has been prohibited.

The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 57-74-9
Molecular formula : $C_{10}H_6Cl_8$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for chlordane (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
409.76	-	5.80	1995	1995	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater and marine organisms. For freshwater organisms, acute and chronic data are present on insects, crustaceans and fish. For marine organisms, chronic data are available on crustaceans and fish and acute data also on molluscs. For organisms which can be regarded as target-species only chronic data are available (part III; appendix D). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity. The lowest NOEC present is $0.015 \mu g/l$ for marine water crustacean. The lowest LC_{50} value is $0.4 \mu g/l$ (Van de Plassche, 1994).

Soil/sediment

Chronic as well as acute toxicity data are available for soil organisms: acute data for oligochaetes, collembola and insects; chronic data for micro-organisms, microbial processes and enzyme activity (part III; appendix D). The lowest LC_{50} is $4.3 mg/kg$ for insects and the lowest NOEC $1.7 mg/kg$ for enzyme activity (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

For mammals only one NOEC of $30 mg/kg$ food for *Rattus norvegicus* is available. For birds only acute data are available: the lowest LC_{50} being $330 mg/kg$ food (part III; appendix D) (Van de Plassche, 1994).

The geometric mean BCF for freshwater and marine water fish is 17,000 l/kg (with a maximum BCF of 38,000 l/kg) (part III; appendix D). The calculated BCF for fish (formula 10) is 30,000 l/kg. The geometric mean BCF for marine water bivalves is 5,400 l/kg (part III; appendix D). The calculated BCF (formula 11) is 8,200 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

Even though no toxicity data are available for algae, the modified EPA method is used to derive the MPC based on direct effects, applying a factor of 10 instead of 1,000 on the lowest LC₅₀. Subsequently this value is compared to the lowest NOEC extrapolated. Finally, the extrapolated NOEC is chosen as the MPC. This is considered acceptable because a considerable amount of NOECs are available for, amongst others, fish, crustaceans and insects. The MPC, based on the combined data sets for marine and freshwater organisms, is 0.0015 µg/l (Van de Plassche, 1994).

Indirect effects

The NEC based on the combined data sets for birds and mammals and calculated with the modified EPA method is 3 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 0.057 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is much higher than the MPC in water based on direct effects, using the geometric mean as well as the maximum BCF. It is concluded that there will probably be no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC for the aquatic environment is set at 0.0015 µg/l (Van de Plassche, 1994). The NC in surface water is $1.5 \cdot 10^{-5}$ µg/l (table 2).

3.2 Soil

Direct effects

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The MPC in soil is 0.0043 mg/kg in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals, and using the BCF for earthworms, is 0.69 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is considerably higher than the MPC in soil based on direct effects. This is also the case if the maximum BCF is used. Therefore there is probably no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC in soil is set at 0.0043 mg/kg, the MPC based on direct effects on terrestrial organisms (Van de Plassche, 1994). The NC in soil is $4.3 \cdot 10^{-5}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6) and is 0.0024 mg/kg (Van de Plassche, 1994). The NC in sediment is $2.4 \cdot 10^{-5}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Final Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.0015	0.0043	0.0080	-
NC	$1.5 \cdot 10^{-5}$	$4.3 \cdot 10^{-5}$	$8.0 \cdot 10^{-5}$	-

4. Harmonization of MPCs and NCs

Because only MPCs for surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.0080 mg/kg) is almost equal to the MPC in soil, based on toxicity data, being 0.0043 mg/kg (table 2). It is decided to set the harmonized MPC in soil equal to the one based on direct effects on soil organisms, i.e. 0.0043 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $0.05 \mu\text{g/m}^3$ and $0.02 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Final Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.0015	0.0043	0.0080	-
NC	$1.5 \cdot 10^{-5}$	$4.3 \cdot 10^{-5}$	$8.0 \cdot 10^{-5}$	-
CritConc	-	-	-	0.05 (air) 0.02 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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CHLORPYRIFOS

1. Introduction

Chlorpyrifos is an organic substance, which is used as an insecticide. It is also used against household pests and the control of ectoparasites on cattle and sheep (Worthing et al., 1991). The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 2921-88-2

Molecular formula : $C_9H_{11}C_{13}N-O_3-P-S$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for chlorpyrifos (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg} ($10^{-6}/s$)	Readily biodegradable	Vp
350.59	-	5.27	380	380	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater and marine organisms. For freshwater organisms, acute data are available on insects, crustaceans and fish and chronic data on protozoa in addition. For marine organisms, many acute data are available on protozoa, algae, crustaceans, molluscs and fish, whilst only chronic data are available on fish (part III; appendix D). Based on this data, marine and freshwater organisms do not seem to differ significantly in sensitivity to chlorpyrifos. The lowest NOEC is 0.012 $\mu g/l$ for freshwater fish (Van de Plassche, 1994).

Soil/sediment

Chronic as well as acute toxicity data are available for soil organisms: acute data for oligochaetes and collembola; chronic data for micro-organisms, oligochaetes, microbial processes and enzyme activity (part III; appendix D). The lowest NOEC is 0.46 mg/kg for enzyme activity and the lowest LC_{50} 0.36 mg/kg for collembola (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

For mammals only one NOEC of 6 mg/kg food for *Rattus norvegicus* is available. For birds the lowest LC_{50} is 190 mg/kg food and the lowest NOEC is 12.5 mg/kg food (part III; appendix D) (Van de Plassche, 1994).

The geometric mean whole body BCF for freshwater and marine water fish is 400 l/kg (with a maximum BCF of 1,700) (part III; appendix D). The calculated BCF for fish (formula 10) is 8,900 l/kg. The difference between calculated and experimental BCFs is probably caused by biotransformation (Deneer, 1993). Experimental BCFs for bivalves are not available. The calculated BCF (formula 11) is 2,400 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

To derive an MPC based on direct effects the method of Aldenberg and Slob is used. This MPC, based on the combined data sets for freshwater and marine organisms, is 0.0028 µg/l (Van de Plassche, 1994).

Indirect effects

The NEC based on the combined data sets for birds and mammals and calculated with the method of Aldenberg and Slob is 3.7 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 3.0 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is higher than the MPC in water based on direct effects, using the geometric mean as well as the maximum BCF. It is therefore concluded that there will probably be no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC for the aquatic environment is set at 0.0028 µg/l (Van de Plassche, 1994). The NC in surface water is $2.8 \cdot 10^{-5}$ µg/l (table 2).

3.2 Soil

Direct effects

The modified EPA method is used to derive an MPC in soil, applying a factor of 1,000 on the lowest LC₅₀. The MPC in soil is $3.6 \cdot 10^{-4}$ mg/kg in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set of birds and mammals (using the BCF for earthworms) is 0.85 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is much higher than the MPC in soil based on direct effects, even if the maximum BCF is used. Therefore, there is probably no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC in soil is set at $3.6 \cdot 10^{-4}$ mg/kg, the MPC based on direct effects (Van de Plassche, 1994). The final NC in soil is $3.6 \cdot 10^{-6}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. The MPC is therefore calculated using the equilibrium partitioning method (formula 6) and is 0.0011 mg/kg (Van de Plassche, 1994). The NC in sediment is $1.1 \cdot 10^{-5}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Final Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.0028	$3.6 \cdot 10^{-4}$	0.0011	-
NC	$2.8 \cdot 10^{-5}$	$3.6 \cdot 10^{-6}$	$1.1 \cdot 10^{-5}$	-

4. Harmonization of MPCs and NCs

Because only MPCs for surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.0011 mg/kg) is somewhat higher than the MPC in soil (based on toxicity data) being $3.6 \cdot 10^{-4} \text{ mg/kg}$ (table 2). The former is preferred because this value is based on a relatively large data set for aquatic organisms (chronic data for 4 taxonomic groups; 19 different species) compared to soil organisms. Thus, it is decided to set the harmonized MPC in soil at 0.0011 mg/kg , based on the equilibrium partitioning method (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $0.07 \mu\text{g/m}^3$ and $0.5 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Final Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.0028	0.0011	0.0011	-
NC	$2.8 \cdot 10^{-5}$	$1.1 \cdot 10^{-5}$	$1.1 \cdot 10^{-5}$	-
CritConc	-	-	-	0.07 (air) 0.5 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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DDD

1. Introduction

(p,p')-DDD is an organic substance and a degradation product of DDT, which was formerly used as an insecticide. In the Netherlands its use has been prohibited. The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 172-54-8

Molecular formula : $C_{14}H_{10}Cl_4$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for DDD (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
320.04	-	6.22	4,074	4,074	-	No	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data are available on freshwater organisms as well as on marine organisms (part III; appendix D). For freshwater organisms many acute data are available on crustaceans, insects, fish, amphibia. No chronic data are available. For marine organisms only acute data are available on algae, crustaceans, molluscs and fish. The lowest LC_{50} value is $2.4 \mu g/l$ for marine crustaceans (Van de Plassche, 1994).

Soil/sediment

No toxicity data for soil organisms or organisms exposed via contaminated sediment are available (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

No toxicity data for mammals are available. The lowest NOEC for birds is 1.1 mg/kg food (Van de Plassche, 1994).

No geometric mean whole body BCFs for marine water and freshwater fish or bivalves are available. The calculated BCF for fish (formula 10) is 80,000 l/kg and for bivalves (formula 11) is 22,000 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC in water based on direct effects is calculated using the modified EPA method. The MPC is $0.0024 \mu\text{g/l}$ using data for marine water as well as freshwater organisms. The lower value for DDD compared to DDT, being $0.0050 \mu\text{g/l}$, is caused by the use of high assessment factors because DDD has been studied to a lesser extent. Since DDT is most toxic to aquatic organisms, it is decided that the MPC in surface water (based on direct effects derived for DDT) should also be the MPC for DDD (Van de Plassche, 1994).

Indirect effects

Combining data sets for birds and mammals and applying the modified EPA method leads for DDD to an indicative NEC of 0.11 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is $4.4 \cdot 10^{-4} \mu\text{g/l}$ for DDD (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is lower than the MPC in water based on direct effects. It can be concluded that there is probably a risk of secondary poisoning via the aquatic route, especially for birds. Thus, the final MPC for the aquatic environment is set at the MPC for secondary poisoning for birds, i.e. $4.4 \cdot 10^{-4} \mu\text{g/l}$ (Van de Plassche, 1994). The final NC in surface water is $4.4 \cdot 10^{-6} \mu\text{g/l}$ (table 2).

3.2 Soil

Direct effects

Because no toxicity data for soil organisms are available for DDD, the equilibrium partitioning method is used for this compound (formula 7) to derive an MPC in soil. The MPC is 0.0018 mg/kg (Van de Plassche, 1994).

Indirect effects

For DDD no MPC for secondary poisoning in the terrestrial food chain is presented due to the absence of data for soil organisms (Van de Plassche, 1994).

Final MPC

For DDD it is proposed to set the final MPC in soil at the one based on direct effects for p,p'-DDT, i.e. 0.010 mg/kg (Van de Plassche, 1994). The final NC in soil is $1.0 \cdot 10^{-4} \text{ mg/kg}$ (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. The MPC is therefore calculated using the equilibrium partitioning method (formula 6) and is 0.0018 mg/kg (Van de Plassche, 1994). The NC in sediment is $1.8 \cdot 10^{-5} \text{ mg/kg}$ (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.4 \cdot 10^{-4}$	0.010	0.0018	-
NC	$4.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$1.8 \cdot 10^{-5}$	-

4. Harmonization of MPCs and NCs

For DDD the harmonized MPC in soil as derived for DDT is used. Because in the case of DDT only MPCs for surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.0094 mg/kg for both isomers of DDT) is almost equal to the MPC in soil, based on toxicity data, being 0.010 mg/kg. It is decided that the harmonized MPC in soil for DDT (and DDD) should be set equal to the MPC based on effects on soil organisms and equilibrium partitioning, i.e. 0.010 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 0.004 $\mu\text{g}/\text{m}^3$ and 0.07 $\mu\text{g}/\text{l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	$4.4 \cdot 10^{-4}$	0.010	0.0018	-
NC	$4.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$1.8 \cdot 10^{-5}$	-
CritConc	-	-	-	0.004 (air) 0.07 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g}/\text{l}$

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DDE

1. Introduction

(p,p')-DDE is an organic substance and a degradation product of DDT, which was formerly used as an insecticide. In the Netherlands its use has been prohibited. The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 72-55-9
Molecular formula : $C_{14}H_8Cl_4$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for DDE (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
318.02	-	6.50	3311	3311	-	No	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 K_p = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as on marine organisms (part III; appendix D). For freshwater organisms only acute data are available on crustaceans, insects, fish, amphibia and flatworms. For marine organisms, chronic data are available on crustaceans and acute data also on molluscs. The lowest NOEC is 0.10 $\mu g/l$ and the lowest LC_{50} 2.5 $\mu g/l$ for marine crustaceans (Van de Plassche, 1994).

Soil/sediment

No toxicity data for soil organisms or organisms exposed via contaminated sediment are available (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

No toxicity data for mammals are available. The lowest NOEC for birds is 0.3 mg/kg food (Van de Plassche, 1994).

The geometric mean whole body BCF for marine water and freshwater fish is 51,000 l/kg. The calculated BCF for DDE (formula 10) is 150,000 l/kg. The available geometric mean BCF for marine water and freshwater bivalves is 118,000 l/kg (with a maximum BCF of 310,000 l/kg) (all values based on field data). The calculated BCF (formula 11) is 41,000 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC in water based on direct effects is calculated via the modified EPA method. The MPC is $0.0025 \mu\text{g/l}$, using data for marine water as well as freshwater organisms. The lower value for DDE compared to DDT, being $0.005 \mu\text{g/l}$, is caused by the use of high assessment factors because this compound has been studied to a lesser extent. Since DDT is the most toxic to aquatic organisms, it is decided that the MPC in surface water (based on direct effects derived for DDT) should also be used for DDE (Van de Plassche, 1994).

Indirect effects

Combining data sets for birds and mammals and applying the method of Aldenberg and Slob results in an MPC of 0.15 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is $9.4 \cdot 10^{-4} \mu\text{g/l}$ (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is lower than the MPC in water based on direct effects. Using the maximum BCF, the MPC is a factor of 2-3 lower. It can be concluded that there is probably a risk of secondary poisoning via the aquatic route, especially for birds. Thus, the final MPC for the aquatic environment is set at the lowest MPC for secondary poisoning for birds. It is decided that the lowest MPC of DDT and its degradation products, DDD and DDE, should be taken, i.e. $4.4 \cdot 10^{-4} \mu\text{g/l}$ (for DDD) (Van de Plassche, 1994). The final NC in surface water is $4.4 \cdot 10^{-6} \mu\text{g/l}$ (table 2).

3.2 Soil

Direct effects

Because no toxicity data for soil organisms are available for DDE, the equilibrium partitioning method is used for this compound (formula 7) to derive an MPC in soil. The MPC is 0.0015 mg/kg (Van de Plassche, 1994).

Indirect effects

For DDE no MPC for secondary poisoning in the terrestrial food chain is presented, due to the absence of ecotoxicity data for soil organisms (Van de Plassche, 1994).

Final MPC

For DDE it is proposed that the final MPC in soil is set at 0.010 mg/kg ; the MPC being based on direct effects for p,p'-DDT (Van de Plassche, 1994). The NC in soil is $1.0 \cdot 10^{-4} \text{ mg/kg}$ (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. The MPC is therefore calculated using the equilibrium partitioning method (formula 6) and is 0.0015 mg/kg (Van de Plassche, 1994). The NC in sediment is $1.5 \cdot 10^{-5} \text{ mg/kg}$ (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.4 \cdot 10^{-4}$	0.010	0.0015	-
NC	$4.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$1.5 \cdot 10^{-5}$	-

4. Harmonization of MPCs and NCs

For DDE it is proposed that the harmonized MPC in soil as derived for DDT be used. Because in the case of DDT only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.0094 mg/kg for both isomers of DDT) is almost equal to 0.010 mg/kg, the MPC in soil, based on toxicity data. It is decided that the harmonized MPC in soil for DDT (and DDE) should be set equal to 0.010 mg/kg; the MPC being based on effects on soil organisms and equilibrium partitioning (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 0.02 $\mu\text{g}/\text{m}^3$ and 0.07 $\mu\text{g}/\text{l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	$4.4 \cdot 10^{-4}$	0.010	0.0015	-
NC	$4.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$1.5 \cdot 10^{-5}$	-
CritConc	-	-	-	0.02 (air) 0.07 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g}/\text{l}$

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DDT

1. Introduction

DDT is an organic substance, existing in the isomers o,p'-DDT and p,p'-DDT. DDT was formerly used as an insecticide. In the Netherlands its use has been prohibited. The substance o,p'-DDT is a minor (up to 30%) constituent of technical DDT, of which p,p'-DDT is the predominant component. DDT has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 50-29-3
Molecular formula : C₁₄H₉Cl₅

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for DDT (Van de Plassche, 1994)

Substance	MW	K _{aw}	log K _{ow}	Kp _{soil}	Kp _{sediment}	k _{deg}	Readily biodegradable	Vp
o,p'-DDT	354.48	-	6.61	21,380	21,380	-	No	-
p,p'-DDT	354.48	-	6.91	21,380	21,380	-	No	-

MW = molecular weight in (g/mol)
K_{aw} = air-water partition coefficient
K_{ow} = octanol-water partition coefficient
Kp = partition coefficient (in l/kg)
k_{deg} = degradation rate constant in air (in 10⁻⁶/s)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as on marine organisms (part III; appendix D). For freshwater organisms chronic data are available on green algae, crustaceans and fish and many acute data on crustaceans, insects, fish and amphibia. For marine organisms, chronic data are available on algae and fish, and acute data on crustaceans, molluscs, algae and fish. The lowest NOEC is 0.05 µg/l for freshwater crustaceans. The lowest LC₅₀ is 0.36 µg/l for marine fish (Van de Plassche, 1994).

Soil/sediment

For o,p'-DDT no toxicity data for soil organisms are available. For p,p'-DDT only one acute study is available: the LC₅₀ is 10 mg/kg for the insect *Gryllus pennsylvanicus* (part III; appendix D). No chronic data are available (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

For o,p'-DDT no toxicity data for mammals are available. For p,p'-DDT a substantial amount of chronic data are available for birds as well as mammals. DDT is considerably more toxic to birds than to mammals; e.g. for p,p'-DDT mean NOECs are 130 and 12 mg/kg food for mammals and birds, respectively. The lowest NOEC for birds is 0.5 and 50 mg/kg food for p,p'-DDT and o,p'-DDT, respectively (Van de Plassche, 1994).

The geometric mean whole body BCFs for marine water and freshwater fish are 37,000 and 52,000 l/kg for o,p'-DDT and p,p'-DDT, respectively. The maximum BCF is 93,000 l/kg for p,p'-DDT. The calculated BCFs for p,p'-DDT and o,p'-DDT (formula 10) are 390,000 and 200,000 l/kg, respectively. The BCF for marine water and freshwater bivalves is 151,000 l/kg for p,p'-DDT (with a maximum BCF of 690,000 l/kg) (all values based on field data). The calculated BCFs (formula 11) are 110,000 and 53,000 l/kg for p,p'-DDT and o,p'-DDT, respectively. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC in water based on direct effects is calculated using the modified EPA method. The MPC is 0.0050 µg/l, using data for marine water as well as freshwater organisms (Van de Plassche, 1994).

Indirect effects

Combining data sets for birds and mammals and applying the method of Aldenberg and Slob leads for p,p'-DDT to a NEC of 0.47 mg/kg food. For o,p'-DDT the NEC based on the modified EPA method is 5 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. The MPCs, based on the combined data set of birds and mammals, are 0.0029 and 0.043 µg/l for p,p'-DDT and o,p'-DDT, respectively (Van de Plassche, 1994).

Final MPC

For p,p'-DDT the MPC for secondary poisoning is lower than the MPC in water based on direct effects. Using the maximum BCF, the MPC is a factor of 2-3 lower. It can be concluded that there is probably a risk of secondary poisoning via the aquatic route, especially for birds. Thus, the final MPC for the aquatic environment is set at the lowest MPC for secondary poisoning for birds. It is decided that the lowest MPC of DDT (and its degradation products DDD and DDE) be taken, i.e. $4.4 \cdot 10^{-4}$ µg/l (for DDD) (Van de Plassche, 1994). The NC in surface water is $4.4 \cdot 10^{-6}$ µg/l (table 2).

3.2 Soil

Direct effects

For p,p'-DDT to derive an MPC in soil the modified EPA method is used, applying a factor of 1,000 on the lowest LC₅₀ for a target species. The MPC for p,p'-DDT is 0.010 mg/kg in standard soil. Because no toxicity data for soil organisms are available for o,p'-DDT, the equilibrium partitioning method is used for this compound (formula 7) to derive an MPC in soil. This MPC is 0.0094 mg/kg (Van de Plassche, 1994).

Indirect effects

For o,p'-DDT no results are presented due to the absence of ecotoxicity data for soil organisms. For p,p'-DDT the MPC for secondary poisoning in the terrestrial food chain, based on the combined data set and calculated with the modified Aldenberg and Slob (using the BCF for earthworms) is 0.11 mg/kg (Van de Plassche, 1994).

Final MPC

For p,p'-DDT the MPC for secondary poisoning is higher than the MPC in soil based on direct effects. Using the maximum BCF the MPC for secondary poisoning based on toxicity data for birds only is slightly lower than the MPC in soil based on direct effects: 0.0048 versus 0.010 mg/kg, respectively. It is remarkable that there seems to be no risk of secondary poisoning even though adverse effects due to biomagnification have been reported in the past for DDT (WHO, 1989^a). The final MPC in soil is set at 0.010 mg/kg, the one based on direct effects (Van de Plassche, 1994). The NC is $1.0 \cdot 10^{-4}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. The MPC is therefore calculated using the equilibrium partitioning method (formula 6) and is 0.0094 mg/kg for DDT (both isomers) (Van de Plassche, 1994). The NC in sediment is $9.4 \cdot 10^{-5}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.4 \cdot 10^{-4}$	0.010	0.0094	-
NC	$4.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$9.4 \cdot 10^{-5}$	-

4. Harmonization of MPCs and NCs

Because for DDT only MPCs for surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.0094 mg/kg for both isomers of DDT) is almost equal to the MPC in soil, based on toxicity data, being 0.010 mg/kg. It is decided that the harmonized MPC in soil for DDT should be set equal to 0.010 mg/kg based on effects on soil organisms and equilibrium partitioning (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $0.001 \mu\text{g/m}^3$ and $0.07 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.4 \cdot 10^{-4}$	0.010	0.0094	-
NC	$4.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$9.4 \cdot 10^{-5}$	-
CritConc	-	-	-	0.001 (water) 0.07 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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ENDOSULFAN

1. Introduction

Endosulfan is an organic substance, which was used as an insecticide and acaricide. In the Netherlands its use has been prohibited. The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 115-29-7

Molecular formula : $C_9H_8Cl_6O_3S$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for endosulfan (Van de Plassche et al., 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
406.91	-	3.83	64.6	64.6	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche et al., 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater organisms as well as on marine organisms (part III; appendix D). For freshwater organisms, chronic data are available on algae, protozoa, crustaceans and fish. For marine organisms, many acute data are available on archiannelids, crustaceans, echinoderms, molluscs and fish. Chronic data are available on relatively insensitive species only, i.e. algae and molluscs. The compound is highly toxic to freshwater fish: the lowest NOEC value is 0.2 $\mu g/l$ for freshwater fish, the lowest LC_{50} value is 0.04 $\mu g/l$ for crustaceans. Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity (Van de Plassche, 1994).

Soil/sediment

Acute and chronic toxicity data are available on organisms exposed via contaminated soil: acute data for oligochaetes; chronic data for microbial processes and plants (part III; appendix D). The lowest NOEC value is 170 mg/kg for microbial processes, the lowest LC_{50} is 5.0 mg/kg for oligochaete (Van de Plassche, 1994).

For sediment-dwelling organisms NOECs are available for two crustaceans and one polychaete. The lowest NOEC is 0.13 mg/kg (Chandler, 1991).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Only acute toxicity data are available for birds, although for mammals many chronic toxicity data are available (part III; appendix D). The lowest LC_{50} for birds is 805 mg/kg food, while the lowest NOEC for mammals is 3.3 mg/kg food (Van de Plassche, 1994).

The whole body BCF for freshwater and marine water fish is 2,800 l/kg (part III; appendix D). The calculated BCF for fish (formula 10) is 330 l/kg. The geometric mean whole body BCF for marine water bivalves is 53 l/kg (with a maximum BCF of 600 l/kg), while the calculated BCF is 88 l/kg (formula 11). BCFs on freshwater organisms are not available. For earthworms a mean and maximum BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC in surface water based on direct effects is calculated using the modified EPA method, although enough chronic data are available to apply the method according to Aldenberg and Slob. The MPC of 0.12 $\mu\text{g/l}$ based on the latter method, however, is higher than several LC_{50} values. The MPC in water based on direct effects is $4.0 \cdot 10^{-4}$ $\mu\text{g/l}$, applying a factor of 100 on the lowest LC_{50} (Van de Plassche, 1994).

Indirect effects

Comparison of the sensitivity of birds and mammals is hampered by the lack of chronic toxicity data for birds. Since there are no chronic toxicity data available on birds, the NEC based on the combined data set is equal to the NEC for mammals. This latter NEC, based on the Aldenberg and Slob method, is 0.68 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on data sets of birds and mammals, is 0.078 $\mu\text{g/l}$ (Van de Plassche, 1994).

Final MPC

Since the MPC for secondary poisoning is much higher than the MPC in water based on direct effects, it can be concluded that there is probably no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. So, the final MPC for the aquatic environment is set at $4.0 \cdot 10^{-4}$ $\mu\text{g/l}$ (Van de Plassche, 1994). The NC in surface water is $4.0 \cdot 10^{-6}$ $\mu\text{g/l}$ (table 2).

3.2 Soil

Direct effect

To derive an MPC in soil based on direct effects the modified EPA method is used, applying a factor of 100 on the lowest $L(E)C_{50}$. The MPC is 0.050 mg/kg in standard soil (Van de Plassche, 1994).

Indirect effect

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set of birds and mammals (using the BCF for earthworms) is 0.16 mg/kg (Van de Plassche, 1994).

Final MPC

Since the MPC for secondary poisoning is higher than the MPC in soil based on direct effects, there is probably no risk of secondary poisoning at the concentration equal to the MPC based on direct effects. Thus the final MPC in soil is set at 0.050 mg/kg, the MPC being based on direct effects on terrestrial organisms (Van de Plassche, 1994). The NC in soil is $5.0 \cdot 10^{-4}$ mg/kg (table 2).

3.3 Sediment

Although some toxicity results are available, the MPC in sediment is calculated using the equilibrium partitioning method (formula 6). The calculated MPC is $2.6 \cdot 10^{-5}$ mg/kg. Comparing this value with the much higher toxicity results for sediment-dwelling organisms, it can be concluded that this MPC is probably on the low side, due to the relatively low K_p used. Because more reliable toxicity studies are not available, it is decided that the MPC in sediment be maintained at $2.6 \cdot 10^{-5}$ mg/kg (Van de Plassche, 1994). The NC in sediment is $2.6 \cdot 10^{-7}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.0 \cdot 10^{-4}$	0.050	$2.6 \cdot 10^{-5}$	-
NC	$4.0 \cdot 10^{-6}$	$5.0 \cdot 10^{-4}$	$2.6 \cdot 10^{-7}$	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning ($2.6 \cdot 10^{-5} \text{ mg/kg}$) is much lower than the MPC in soil, based on toxicity data, being 0.05 mg/kg . This is caused by the extreme sensitivity of fish, compared to soil organisms, and the relatively low K_p . For the terrestrial environment the MPC in soil based on toxicity data is therefore preferred. Thus, the harmonized MPC in soil is set at 0.05 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $12 \mu\text{g/m}^3$ and $46 \mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.0 \cdot 10^{-4}$	0.050	$2.6 \cdot 10^{-5}$	-
NC	$4.0 \cdot 10^{-6}$	$5.0 \cdot 10^{-4}$	$2.6 \cdot 10^{-7}$	-
CritConc	-	-	-	12 (air) 46 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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ENDRIN

1. Introduction

Endrin is an organic substance, which was formerly used as an insecticide. In the Netherlands its use has been prohibited. The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 72-20-8
Molecular formula : $C_{12}H_8Cl_6O$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for endrin (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
380.90	-	5.20	977	977	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 K_p = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater and marine organisms. For freshwater organisms, acute data are available on crustaceans, insects, fish and amphibia, and chronic data on blue-green algae and fish. For marine organisms, many chronic data are available on algae, crustaceans, molluscs and fish and acute data also on echinoderms (part III; appendix D). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity. One extremely sensitive species is the crustacean, *Penaeus duorarum*, with an LC_{50} of $0.037 \mu g/l$. The lowest NOEC value is $0.03 \mu g/l$ for marine water crustaceans (Van de Plassche, 1994).

Soil/sediment

Only one acute toxicity study is available on organisms exposed via contaminated soil: the lowest LC_{50} is $0.95 mg/kg$ for *Folsomia candida*, being a relatively sensitive organism for insecticides. No chronic data have been found (part III; appendix D) (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Many chronic toxicity data are available for mammals as well as for birds (part III; appendix D). Birds and mammals seem to be equally sensitive. The lowest NOEC is $0.25 mg/kg$ food for birds (Van de Plassche, 1994).

The geometric mean whole body BCF for freshwater and marine water fish is $4,300 l/kg$ (with a maximum BCF of $12,000 l/kg$) (part III; appendix D). The calculated BCF (formula 10) is $7,600 l/kg$. The geometric mean BCF for marine water bivalves is $1,800 l/kg$ (with a maximum BCF of $1,900 l/kg$), whilst the calculated BCF is $2,100 l/kg$ (formula 11) (part III; appendix D). BCFs on freshwater organisms are not available. For earthworms a mean BCF of $1 l/kg$ (with a maximum BCF of $10 l/kg$) is assumed (Van de Plassche, 1994).

endrin

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

Enough NOECs are available to apply the method of Aldenberg and Slob. However, the Kolmogorov-Smirnov $D \cdot \sqrt{n}$ test (part III; appendix D) rejected the distribution of NOECs as being log-logistic at a significant level of 1%. Based on the working-mechanism of endrin, no values can be left out. Therefore, the modified EPA method is applied, using a factor of 10 on the lowest NOEC. The MPC based on direct effects, calculated using the modified EPA method does not differ much from the MPC using the method of Aldenberg and Slob: 0.0030 versus 0.0045 $\mu\text{g/l}$, respectively (Van de Plassche, 1994).

Indirect effects

Combining data sets for birds and mammals and applying the method of Aldenberg and Slob results in a NEC of 0.085 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 0.0063 $\mu\text{g/l}$ (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is higher than the MPC in water based on direct effects. If the maximum BCF is used, the opposite conclusion must be drawn. It can be concluded that there is probably no risk of secondary poisoning via the aquatic route at a concentration equal to the MPC based on direct effects. Thus, the final MPC for the aquatic environment is set at 0.0030 $\mu\text{g/l}$ (Van de Plassche, 1994). The NC in surface water is $3.0 \cdot 10^{-5}$ $\mu\text{g/l}$ (table 2).

3.2 Soil

Direct effects

To derive an MPC in soil based on direct effects the modified EPA method is used, applying a factor of 1,000 on the lowest LC₅₀. The MPC is $9.5 \cdot 10^{-4}$ mg/kg in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals, using the BCF for earthworms, is 0.020 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is much higher than the MPC in soil based on direct effects; also if the maximum BCF is used. Therefore there is probably no risk of secondary poisoning at the concentration equal to the MPC based on direct effects. Thus, the final MPC in soil is set at $9.5 \cdot 10^{-4}$ mg/kg (Van de Plassche, 1994). The NC in soil is $9.5 \cdot 10^{-6}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6) and is 0.0029 mg/kg (Van de Plassche, 1994). The NC in sediment is $2.9 \cdot 10^{-5}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.0030	$9.5 \cdot 10^{-4}$	0.0029	-
NC	$3.0 \cdot 10^{-5}$	$9.5 \cdot 10^{-6}$	$2.9 \cdot 10^{-5}$	-

4. Harmonization of MPCs en NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (i.e. 0.0029 mg/kg) is higher than the MPC in soil, based on toxicity data, being $9.5 \cdot 10^{-4}$ mg/kg . The MPC value based on equilibrium partitioning is preferred, however, because for aquatic organisms much more toxicity data are available than for terrestrial organisms. It is decided to set the harmonized MPC in soil equal to the MPC based on the equilibrium partitioning method, i.e. 0.0029 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 0.0002 $\mu\text{g/m}^3$ and 0.02 $\mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of harmonized Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.0030	0.0029	0.0029	-
NC	$3.0 \cdot 10^{-5}$	$2.9 \cdot 10^{-5}$	$2.9 \cdot 10^{-5}$	-
CritConc	-	-	-	0.0002 (air) 0.02 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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FENTHION

1. Introduction

Fenthion is an organic substance which is used as an insecticide with a useful penetrant and persistent action (Worthing et al., 1991). The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 55-38-9
Molecular formula : $C_{10}H_{15}O_3PS_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for fenthion (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
278.34	-	4.09	112	112	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater and marine organisms. For freshwater organisms, acute data are available on insects, molluscs, crustaceans, fish and amphibia and chronic data on protozoans and molluscs. For marine organisms, acute data are available on algae, crustaceans, insects, molluscs and fish and chronic data on algae and crustaceans (part III; appendix D). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity to fenthion. The variation in chronic data available is large. The lowest NOEC present is $0.037 \mu g/l$ for marine water crustacean. One marine water crustacean, *Penaeus spec.*, is extremely sensitive to fenthion: the lowest LC_{50} value is $0.024 \mu g/l$ (Van de Plassche, 1994).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

For birds only acute data are available; the lowest LC_{50} is 3 mg/kg food. For mammals only one NOEC is available: 0.13 mg/kg food (part III; appendix D) (Van de Plassche, 1994).

Only one experimental BCF is available from a study with exposure of freshwater fish to a mixture of seven compounds. The BCF is 170 l/kg (part III; appendix D). The calculated BCF for fish (formula 10) is 590 l/kg, and the one for bivalves (formula 11) is 160 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC based on direct effects, calculated using the method of Aldenberg and Slob, is 0.0031 $\mu\text{g/l}$ (based on the combined data sets for marine and freshwater organisms) (Van de Plassche, 1994).

Indirect effects

The MPC for birds and mammals based on the modified EPA method is 0.013 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for bivalves (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 0.016 $\mu\text{g/l}$ (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is considerably higher than the MPC in water based on direct effects, indicating that there will probably be no risk of secondary poisoning via the aquatic route. Thus, the final MPC for the aquatic environment is set at 0.0031 $\mu\text{g/l}$ (Van de Plassche, 1994). The NC in surface water is $3.1 \cdot 10^{-5}$ $\mu\text{g/l}$ (table 2).

3.2 Soil

Because no toxicity data for soil organisms are available the equilibrium partitioning method is used (formula 7) to derive an MPC in soil. This MPC is $3.5 \cdot 10^{-4}$ mg/kg (Van de Plassche, 1994). The NC in soil is $3.5 \cdot 10^{-6}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6) and is $3.5 \cdot 10^{-4}$ mg/kg (Van de Plassche, 1994). The NC in sediment is $3.5 \cdot 10^{-6}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.0031	$3.5 \cdot 10^{-4}$	$3.5 \cdot 10^{-4}$	-
NC	$3.1 \cdot 10^{-5}$	$3.5 \cdot 10^{-6}$	$3.5 \cdot 10^{-6}$	-

4. Harmonization of MPCs and NCs

Since no toxicity data are available for soil and sediment-dwelling organisms and consequently the MPC in soil is calculated by equilibrium partitioning, harmonization of MPCs for the different compartments is not necessary. In this case, the MPC in soil based on equilibrium partitioning is compared to the ratio of the lowest NOEC for birds/mammals and the mean BCF for earthworms. For fenthion the lowest NOEC/BCF for birds and mammals of 0.030 mg/kg is considerably higher than the MPC in soil calculated by equilibrium partitioning, being $3.5 \cdot 10^{-4}$ mg/kg. The value of $3.5 \cdot 10^{-4}$ mg/kg seems therefore reasonably 'safe' with respect to adverse effects due to secondary poisoning. It is decided to set the MPC in soil at $3.5 \cdot 10^{-4}$ mg/kg (Van de Plassche, 1994).

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For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $0.0005 \mu\text{g}/\text{m}^3$ and $0.06 \mu\text{g}/\text{l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	0.0031	$3.5 \cdot 10^{-4}$	$3.5 \cdot 10^{-4}$	-
NC	$3.1 \cdot 10^{-5}$	$3.5 \cdot 10^{-6}$	$3.5 \cdot 10^{-6}$	-
CritConc	-	-	-	0.0005 (air) 0.06 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g}/\text{l}$

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α -HCH

1. Introduction

α -HCH is an organic substance which is used as an insecticide. The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 319-84-6

Molecular formula : $C_6H_6Cl_6$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for α -HCH (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
290.82	-	3.78	89	89	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are available on freshwater and marine organisms. For freshwater organisms, only chronic data are present on green algae, protozoans, molluscs, crustaceans and fish. For marine organisms, acute data are available on crustaceans and fish and chronic data on algae and fish (part III; appendix D). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity. The lowest NOEC present is 9 $\mu g/l$ for protozoans (Van de Plassche, 1994).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

No toxicity data are available for birds, whilst for mammals only two NOECs are available, the lowest NOEC is 50 mg/kg food (part III; appendix D) (Van de Plassche, 1994).

The geometric mean whole BCF for marine and freshwater fish is 650 l/kg (with a maximum BCF of 1,200 l/kg) (part III; appendix D). The calculated BCF for fish (formula 10) is 290 l/kg, and the one for bivalves (formula 11) is 78 l/kg. Only one experimental BCF for bivalves is available, being 160 l/kg (part III; appendix D). For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC based on the combined data set for marine and freshwater organisms and calculated using the method of Aldenberg and Slob, is $3.5 \mu\text{g/l}$ (Van de Plassche, 1994). This MPC is a of factor 2-3 lower than the lowest NOEC.

Indirect effects

Comparison of the sensitivity of birds and mammals is hampered by the lack of toxicity data for birds. The MPC based on the combined data set for birds and mammals is set at 5 mg/kg food, the MPC for mammals, based on the modified EPA method (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is $2.5 \mu\text{g/l}$ (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning based on the BCF is only slightly lower than the MPC in water based on direct effects. If the maximum BCF is used, the MPC for secondary poisoning is lower than the one based on direct effects. It is decided to set the final MPC for the aquatic environment at $2.5 \mu\text{g/l}$, because there might be a risk of secondary poisoning (Van de Plassche, 1994). The NC in surface water $0.025 \mu\text{g/l}$ (table 2).

3.2 Soil

Because no toxicity data for soil organisms are available, the equilibrium partitioning method is used (formula 7) to derive an MPC in soil. This MPC is 0.22 mg/kg (Van de Plassche, 1994). The NC in soil is $2.2 \cdot 10^{-3} \text{ mg/kg}$ (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore an MPC of 0.22 mg/kg is calculated using the equilibrium partitioning method (formula 6) (Van de Plassche, 1994). The NC in sediment is $2.2 \cdot 10^{-3} \text{ mg/kg}$ (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	2.5	0.22	0.22	-
NC	0.025	$2.2 \cdot 10^{-3}$	$2.2 \cdot 10^{-3}$	-

4. Harmonization of MPCs and NCs

Since no toxicity data are available for soil and sediment-dwelling organisms and, consequently, the MPC in soil is calculated by equilibrium partitioning, harmonization of MPCs for the different compartments is not necessary. In this case, the MPC in soil based on equilibrium partitioning is compared to the ratio of the lowest NOEC for birds/mammals and the mean BCF for earthworms. The lowest NOEC/BCF for mammals (data for birds are not available) of 1.2 mg/kg is higher than the MPC in soil calculated by equilibrium partitioning, being 0.22 mg/kg . Using the maximum BCF, the MPC based on equilibrium partitioning is higher. Based on these data the value of 0.22 mg/kg seems therefore reasonably 'safe' with respect to adverse effects due to secondary poisoning. The MPC in soil is therefore set at 0.22 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $12 \mu\text{g}/\text{m}^3$ and $34 \mu\text{g}/\text{l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	2.5	0.22	0.22	-
NC	0.025	$2.2 \cdot 10^{-3}$	$2.2 \cdot 10^{-3}$	-
CritConc	-	-	-	12 (air) 34 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g}/\text{l}$

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β -HCH

1. Introduction

β -HCH is an organic substance, which is used as an insecticide. The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 319-85-7

Molecular formula : $C_6H_6Cl_6$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for β -HCH (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
290.82	-	3.84	1148	1148	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Only chronic toxicity data are available on freshwater and marine organisms. For freshwater organisms, data are available on green algae, protozoans, crustaceans and fish. For marine organisms one NOEC is available on crustaceans (part III; appendix D). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity. The lowest NOEC is 10 $\mu g/l$ for marine crustacean (Van de Plassche, 1994).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Chronic toxicity data for birds and mammals are scarce. β -HCH may be more toxic to mammals than the other HCH-isomers. This is possibly caused by an effect on the endocrine organs: an estrogenic potency has been shown (IPCS, 1992). The lowest NOEC for mammals is 2 mg/kg food; the only available NOEC for birds is ≥ 630 mg/kg food (part III; appendix D) (Van de Plassche, 1994).

The geometric mean whole body BCF for freshwater fish is 800 l/kg (with a maximum BCF of 1,500 l/kg). For marine fish no experimental BCF is available (part III; appendix D). The calculated BCF for fish (formula 10) is 330 l/kg, and the one for bivalves (formula 11) is 90 l/kg. Only one experimental BCF for bivalves is available, being 130 l/kg (part III; appendix D). For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC based on the combined data set for marine and freshwater organisms and calculated using the method of Aldenberg and Slob, is 6.1 µg/l (Van de Plassche, 1994).

Indirect effects

Comparison of the sensitivity of birds and mammals to β-HCH is hampered by the lack of sufficient toxicity data for birds. The MPC based on the combined data set for birds and mammals is set equal to the MPC for mammals, based on the modified EPA method: 0.2 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 0.080 µg/l (Van de Plassche, 1994).

Final MPC

The low NOEC value for mammals leads to an MPC for secondary poisoning being lower than the MPC in water based on direct effects; the same is true if the maximum BCF is used. It can therefore be concluded that, because there might be a risk of secondary poisoning, the final MPC for the aquatic environment is set at 0.080 µg/l (Van de Plassche, 1994). The NC in surface water is $8.0 \cdot 10^{-4}$ µg/l (table 2).

3.2 Soil

Because no toxicity data for soil organisms are available, the equilibrium partitioning method is used (formula 7) to derive an MPC in soil. This MPC is 0.092 mg/kg (Van de Plassche, 1994). The NC in soil is $9.2 \cdot 10^{-4}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore an MPC of 0.092 mg/kg is calculated using the equilibrium partitioning method (formula 6) (Van de Plassche, 1994). The NC in sediment is $9.2 \cdot 10^{-4}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	0.080	0.092	0.092	-
NC	$8.0 \cdot 10^{-4}$	$9.2 \cdot 10^{-4}$	$9.2 \cdot 10^{-4}$	-

4. Harmonization of MPCs and NCs

Since no toxicity data are available for soil and sediment-dwelling organisms and, consequently, the MPC in soil is calculated by equilibrium partitioning, harmonization of MPCs for the different compartments is not necessary. In this case the MPC in soil based on equilibrium partitioning is compared to the ratio of the lowest NOEC for birds/mammals and the mean BCF for earthworms. The lowest NOEC/BCF for birds and mammals of 0.46 mg/kg is a factor of 5 higher than the MPC in soil calculated by equilibrium partitioning, being 0.092 mg/kg. If the maximum BCF is used, the NOEC/BCF value is a factor of 2 lower. Based on these data the value of 0.092 mg/kg seems reasonably 'safe' with respect to adverse effects due to secondary poisoning. It is decided to set the MPC in soil at 0.092 mg/kg (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $0.77 \mu\text{g}/\text{m}^3$ and $15 \mu\text{g}/\text{l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	0.080	0.092	0.092	-
NC	$8.0 \cdot 10^{-4}$	$9.2 \cdot 10^{-4}$	$9.2 \cdot 10^{-4}$	-
CritConc	-	-	-	0.77 (air) 15 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g}/\text{l}$

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HEPTACHLOR AND HEPTACHLOR EPOXIDE

1. Introduction

Heptachlor and heptachlor epoxide are organic substances, which were formerly used as pesticides. In the Netherlands their use has been prohibited. Heptachlor epoxide is a persistent degradation product of heptachlor. Heptachlor is converted to heptachlor epoxide in surface water as well as mammals. Both compounds have a similar toxicity (WHO, 1984). Therefore all MPCs for heptachlor epoxide are set equal to the MPCs for heptachlor (except for the MPC in sediment). Consequently, only toxicity data for heptachlor are discussed in this report, while the data for both compounds are presented in appendix D of part III. Both compounds have the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no.	: 76-44-8 (heptachlor)	1024-57-3 (heptachlor epoxide)
Molecular formula	: $C_{10}H_5Cl_7$	$C_{10}H_5Cl_7O$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for heptachlor and heptachlor epoxide (Van de Plassche, 1994)

Substance	MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
Heptachlor	373.30	-	5.58	1413	1413	-	-	-
Heptachlor epoxide	389.30	-	3.49	44	44	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche et al., 1994).

2.2 Ecotoxicity data

Surface water

Many acute toxicity data of heptachlor are available for freshwater organisms (crustaceans, insects, fish and amphibia) and marine organisms (algae, crustaceans, molluscs and fish). Chronic data are available only for freshwater organisms (crustaceans and fish) (part III; appendix D). Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity to heptachlor. The lowest NOEC is $0.86 \mu g/l$ for fish. The lowest LC_{50} value is $0.046 \mu g/l$ for marine crustaceans (Van de Plassche, 1994).

Soil/sediment

Only acute toxicity data are available on organisms exposed via contaminated soil (oligochaetes, collembola and insects) (part III; appendix D). The lowest LC_{50} value of heptachlor is $0.7 mg/kg$ (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Chronic toxicity data for mammals and birds are scarce (part III; appendix D). Only one NOEC is available for both groups, being 50 mg/kg food for Japanese quail and 6 mg/kg food for mammals (Van de Plassche, 1994).

The geometric mean whole body BCF for marine water and freshwater fish is 5,800 l/kg (with a maximum BCF of 9,500 l/kg) (part III; appendix D). The calculated BCF for heptachlor (formula 10) is 18,000 l/kg. The geometric mean BCF for marine water bivalves is 6,300 l/kg, while the calculated BCF is 4,900 l/kg (formula 11) (part III; appendix D). An experimental BCF for freshwater bivalves is not available. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC in surface water based on direct effects is calculated using the modified EPA method applying a factor of 100 on the lowest LC_{50} for heptachlor. This MPC is $4.6 \cdot 10^{-4} \mu g/l$ (Van de Plassche, 1994).

Indirect effects

The MPC based on the combined data set for birds and mammals is set at 0.6 mg/kg food, i.e. the MPC for mammals, calculated with the modified EPA method (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for bivalves (most critical route) is used. The MPC, based on the combined data set of birds and mammals, is $0.019 \mu g/l$ (Van de Plassche, 1994).

Final MPC

Since the MPC for secondary poisoning using the BCF of bivalves is higher than the MPC based on direct effects, there will probably be no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC for the aquatic environment is set at $4.6 \cdot 10^{-4} \mu g/l$ (Van de Plassche, 1994). The NC in surface water is $4.6 \cdot 10^{-6} \mu g/l$ (table 2).

3.2 Soil

Direct effects

To derive an MPC in soil based on direct effects the modified EPA method is used, applying a factor of 1,000 on the lowest LC_{50} value for heptachlor. The MPC is $7.0 \cdot 10^{-4} mg/kg$ in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain can be calculated, incorporating effects on birds and mammals due to secondary poisoning (using the BCF for earthworms). This MPC is 0.14 mg/kg (Van de Plassche, 1994).

Final MPC

Since the MPC for secondary poisoning is much higher than the MPC in soil based on direct effects, there is probably no risk of secondary poisoning at the concentration equal to the MPC based on direct effects. Thus, the final MPC in soil is set at $7.0 \cdot 10^{-4} mg/kg$ based on direct effects on terrestrial organisms (Van de Plassche, 1994). The final NC in soil is $7.0 \cdot 10^{-6} mg/kg$ (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPCs for heptachlor and heptachlor epoxide are calculated using the equilibrium partitioning method (formula 6) and are $6.5 \cdot 10^{-4} mg/kg$ and $2.0 \cdot 10^{-5} mg/kg$, respectively (Van de Plassche, 1994). The NCs are $6.5 \cdot 10^{-6} mg/kg$ and $2.0 \cdot 10^{-7} mg/kg$, respectively.

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.6 \cdot 10^{-4}$ (heptachlor and heptachlor epoxide)	$7.0 \cdot 10^{-4}$ (heptachlor and heptachlor epoxide)	$6.5 \cdot 10^{-4}$ (heptachlor) $2.0 \cdot 10^{-5}$ (heptachlor epoxide)	-
NC	$4.6 \cdot 10^{-6}$ (heptachlor and heptachlor epoxide)	$7.0 \cdot 10^{-6}$ (heptachlor and heptachlor epoxide)	$6.5 \cdot 10^{-6}$ (heptachlor) $2.0 \cdot 10^{-7}$ (heptachlor epoxide)	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPCs calculated by equilibrium partitioning (i.e. $6.5 \cdot 10^{-4}$ mg/kg for heptachlor and $2.0 \cdot 10^{-5}$ mg/kg for heptachlor epoxide) are both lower than the MPC in soil based on toxicity data, being $7.0 \cdot 10^{-4}$ mg/kg . The value of $2.0 \cdot 10^{-5}$ mg/kg (for heptachlor epoxide) is a factor of 35 lower than the MPC in soil. Several factors may be responsible for this large difference, e.g. the uncertainty over the relatively low K_p of 44 l/kg , or characteristics of tests with soil organisms. On the one hand it can be argued that concentrations in pore-water above the MPC for aquatic organisms may cause adverse effects. On the other hand terrestrial toxicity data are available for target organisms. It is decided to set the harmonized MPC in soil equal to $7.0 \cdot 10^{-4}$ mg/kg , the MPC based on direct effects on soil organisms (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 0.2 $\mu\text{g/m}^3$ and 0.02 $\mu\text{g/l}$ (heptachlor) and 0.02 $\mu\text{g/m}^3$ and 0.02 $\mu\text{g/l}$ (heptachlor epoxide), respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	$4.6 \cdot 10^{-4}$ (heptachlor and heptachlor epoxide)	$7.0 \cdot 10^{-4}$ (heptachlor and heptachlor epoxide)	$6.5 \cdot 10^{-4}$ (heptachlor) $2.0 \cdot 10^{-5}$ (heptachlor epoxide)	-
NC	$4.6 \cdot 10^{-6}$ (heptachlor and heptachlor epoxide)	$7.0 \cdot 10^{-6}$ (heptachlor and heptachlor epoxide)	$6.5 \cdot 10^{-6}$ (heptachlor) $2.0 \cdot 10^{-7}$ (heptachlor epoxide)	-
CritConc	-	-	-	0.2 (heptachlor, air) 0.02 (heptachlor epoxide, air) 0.02 ¹⁾ (heptachlor, rainwater) 0.02 ¹⁾ (heptachlor epoxide, rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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LINDANE

1. Introduction

Lindane (γ -HCH) is an organic substance which is used as an insecticide through contact, and has some fumigant action (Worthing and Hance, 1991). The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 608-73-1

Molecular formula : $C_6H_6Cl_6$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for lindane (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
290.85	-	3.69	251	251	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Many chronic toxicity data of lindane are available on freshwater and marine organisms. For freshwater organisms, data are available on blue and green algae, protozoa, molluscs, crustaceans, insects and fish (part III; appendix D). Crustaceans, insects and fish seem to be more sensitive than the other groups. Based on the data available, marine and freshwater organisms do not seem to differ significantly in sensitivity. The lowest NOEC available is 2.2 $\mu g/l$ for freshwater insects (Emans et al., 1992; Van de Plassche, 1994).

Soil/sediment

Chronic as well as acute toxicity data are available for the following soil organisms: collembola and oligochaetes (part III; appendix D). The lowest NOEC is 0.05 mg/kg for collembola (Van de Meent et al., 1990; Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Two and three NOECs are available for birds and mammals, respectively (part III; appendix D). One NOEC value for birds of 1.6 mg/kg food, is 63 and 16 times lower than the next NOEC for birds and the lowest NOEC for mammals, respectively. Based on these data the fact that birds are more sensitive than mammals cannot be ignored (Romijn et al., 1993; Van de Plassche, 1994).

The geometric mean whole body BCF for freshwater and marine fish is 480 l/kg (with a maximum BCF of 1,600 l/kg) (part III; appendix D). The calculated BCF for fish (formula 10) is 240 l/kg. The only available experimental BCF for bivalves is 200 l/kg (part III; appendix D). The calculated BCF for bivalves (formula 11) is 64 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Romijn et al., 1993; Van de Plassche, 1994).

lindane

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

The MPC based on direct effects is calculated using the method of Aldenberg and Slob based on the combined data set for freshwater and marine organisms. This MPC is $1.0 \mu\text{g/l}$ (Van de Plassche, 1994).

Indirect effects

The NEC, based on the combined data set for birds and mammals and calculated with the method of Aldenberg and Slob, is 1.2 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is $0.77 \mu\text{g/l}$ (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is slightly lower than the MPC in water based on direct effects. Using the maximum BCF this value is a factor of between 2-4 lower. It is concluded that there may be a risk of secondary poisoning. Thus, the final MPC for the aquatic environment is set at $0.77 \mu\text{g/l}$ (Van de Plassche, 1994). The NC is $7.7 \cdot 10^{-3} \mu\text{g/l}$ (table 2).

3.2 Soil

Direct effects

The modified EPA method is used to derive an MPC in soil based on direct effects, applying a factor of 10 on the lowest NOEC. This MPC is 0.0050 mg/kg in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals and calculated with the method of Aldenberg and Slob (using the BCF for earthworms) is 0.27 mg/kg (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is higher than the MPC in soil based on direct effects; the same is true if the maximum BCF is used. This indicates that there is probably no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC in soil is set at 0.0050 mg/kg , the MPC based on direct effects on terrestrial organisms (Van de Plassche, 1994). The NC is $5.0 \cdot 10^{-5} \text{ mg/kg}$ (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6) and is 0.19 mg/kg (Van de Plassche, 1994). The NC is 0.0019 mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Final Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.77	0.0050	0.19	-
NC	$7.7 \cdot 10^{-3}$	$5.0 \cdot 10^{-5}$	0.0019	-

4. Harmonization of MPCs and NCs

Because only MPCs in surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. The MPC calculated by equilibrium partitioning (0.19 mg/kg) is much higher than the MPC in soil based on toxicity data, being 0.005 mg/kg . This value is considerably higher than the lowest NOEC for soil organisms. It is therefore decided to set the harmonized MPC in soil equal to 0.005 mg/kg , the MPC based on direct effects on soil organisms (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are 0.01 $\mu\text{g/m}^3$ and 0.25 $\mu\text{g/l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 3: Final Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.77	0.0050	0.19	-
NC	$7.7 \cdot 10^{-3}$	$5.0 \cdot 10^{-5}$	0.0019	-
CritConc	-	-	-	0.01 (air) 0.25 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g/l}$

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QUINTOZENE

1. Introduction

Quintozene is an organic substance which is used as a fungicide. The compound has the potential to bioaccumulate. For deriving MPCs, secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 82-68-8
Molecular formula : $C_6Cl_5-N-O_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for quintozene (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
295.32	-	5.50	1148	1148	-	-	-

MW = molecular weight (in g/mol)
 K_{aw} = air-water partition coefficient
 K_{ow} = octanol-water partition coefficient
 Kp = partition coefficient (in l/kg)
 k_{deg} = degradation rate constant in air (in $10^{-6}/s$)
Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Only acute toxicity data for quintozene are available on freshwater organisms (fish) and none on marine organisms (part III; appendix D). The lowest LC_{50} is 290 $\mu g/l$ for fish (Van de Plassche, 1994).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Only one NOEC is available for birds as well as mammals, being 100 and 25 mg/kg food, respectively (part III; appendix D) (Van de Plassche, 1994).

The whole body BCF for freshwater fish is 240 l/kg (part III; appendix D). For marine water fish no BCF is available. The calculated BCF for fish (formula 10) is 15,000 l/kg. The difference between calculated and experimental BCFs is probably caused by biotransformation (Bahig et al., 1981). Experimental BCFs for bivalves are not available. The calculated BCF (formula 11) is 4,100 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

To derive an MPC based on direct effects the modified EPA method is used, applying a factor of 1,000 on the lowest LC₅₀. This MPC based on data for freshwater fish, is 0.29 µg/l (Van de Plassche, 1994).

Indirect effects

The MPC based on the combined data sets for birds and mammals is set equal to the MPC for mammals and is calculated using the modified EPA method: 2.5 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. The calculated BCF for bivalves is not used, because this is an overestimation of the BCF. The MPC for secondary poisoning based on the combined data set of birds and mammals (using the modified EPA method) is set equal to 3.3 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is higher than the MPC in water based on direct effects, indicating that there will probably be no risk of secondary poisoning via the aquatic route. Thus, the final MPC for the aquatic environment is set at 0.29 µg/l (Van de Plassche, 1994). The final NC in surface water is $2.9 \cdot 10^{-3}$ µg/l (table 2).

3.2 Soil

Because no toxicity data for soil organisms are available the equilibrium partitioning method is used (formula 7) to derive an MPC in soil. This MPC is 0.33 mg/kg (Van de Plassche, 1994). The NC in soil is $3.3 \cdot 10^{-3}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are available for sediment-dwelling organisms. Therefore an MPC of 0.33 mg/kg is calculated using the equilibrium partitioning method (formula 6) (Van de Plassche, 1994). The NC in sediment is $3.3 \cdot 10^{-3}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m ³)
MPC	0.29	0.33	0.33	-
NC	$2.9 \cdot 10^{-3}$	$3.3 \cdot 10^{-3}$	$3.3 \cdot 10^{-3}$	-

4. Harmonization of MPCs and NCs

Since no toxicity data are available for soil and sediment-dwelling organisms and, consequently, the MPC in soil is calculated by equilibrium partitioning, harmonization of MPCs for the different compartments is not necessary. In this case, the MPC in soil based on equilibrium partitioning, is compared to the ratio of the lowest NOEC for birds/mammals and the mean BCF for earthworms. The lowest NOEC/BCF for birds and mammals of 5 mg/kg is higher than the MPC in soil calculated by equilibrium partitioning, being 0.33 mg/kg. The value of 0.33 mg/kg seems therefore reasonably 'safe' with respect to adverse effects due to secondary poisoning: this value is even lower than the NOEC/BCF_{max}. It is therefore decided to set the MPC in soil at 0.33 mg/kg.

quintozene

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $740 \mu\text{g}/\text{m}^3$ and $2.6 \mu\text{g}/\text{l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 2: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	0.29	0.33	0.33	-
NC	$2.9 \cdot 10^{-3}$	$33 \cdot 10^{-3}$	$3.3 \cdot 10^{-3}$	-
CritConc	-	-	-	740 (air) 2.6 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g}/\text{l}$

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TBTO

1. Introduction

TBTO (tributyltin oxide) is one of the tributyltin (TBT) compounds. It is mainly used as an antifouling agent. For the derivation of harmonized MPCs and NCs, the bioaccumulation potential of this compound has not been studied yet.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 56-34-9

Molecular formula : $C_{24}H_{54}O-Sn_2$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for TBTO (Van de Meent et al., 1990)

MW	K_{aw}	$\log K_{ow}$	$K_{p_{soil}}$	$K_{p_{sediment}}$	k_{deg}	Readily biodegradable	Vp
596.16	-	3.85	1,000	1,000	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

K_p = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (K_p s) for soil and sediment are equal (Van de Meent et al., 1990).

2.2 Ecotoxicity data

Surface water

The toxicity data presented apply to tributyltin compounds. The data are available mainly on marine organisms. For freshwater organisms chronic data are available on crustaceans, molluscs and fish. For marine organisms chronic data are available on bacteria, algae, molluscs, crustaceans, worms and fish (part III; appendix D). There are no distinct differences in susceptibility to the compound between freshwater and marine species. The lowest NOEC value is $0.001 \mu g/l$ for marine molluscs (Janus et al., 1994).

Soil/sediment

No toxicity data are available on organisms exposed via contaminated soil or sediment (Janus et al., 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

The MPC in surface water is calculated using the method of Aldenberg and Slob, based on the total data set of 13 values for freshwater and marine organisms. This MPC is $0.003 \mu g/l$, the NC is $3.0 \cdot 10^{-5} \mu g/l$ (table 2) (Janus et al., 1994).

3.2 Soil

Since no toxicity data are present for soil organisms, the MPC is calculated using the equilibrium partitioning method (formula 7) and is $0.003 mg/kg$. The NC is $3.0 \cdot 10^{-5} mg/kg$ (table 2) (Janus et al., 1994; Van de Meent et al., 1990).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore the MPC is calculated using the equilibrium partitioning method (formula 6). Since the K_p for sediment is equal to the K_p for soil, the MPC and NC in sediment are equal to the MPC and NC in soil and are 0.003 mg/kg and $3.0 \cdot 10^{-5}$ mg/kg, respectively (table 2) (Janus et al., 1994; Van de Meent et al., 1990).

3.4 Air

No MPC in air has been derived yet.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water ($\mu\text{g/l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g/m}^3$)
MPC	0.003	0.003	0.003	-
NC	$3.0 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$	-

4. Harmonization of MPCs and NCs

Because the EP method is used as an indirect method to derive an MPC and NC in soil and sediment, the harmonization procedure using the EP method is meaningless.

THIRAM

1. Introduction

Thiram is an organic substance which is used as a fungicide. The compound has the potential to bioaccumulate. For deriving MPCs secondary poisoning via the aquatic and terrestrial route has been taken into account.

2. Data evaluation

2.1 Identification and physico-chemical data

CAS no. : 137-26-8

Molecular formula : $C_6H_{12}N_2S_4$

The physico-chemical data used in the derivation of harmonized MPCs are presented in table 1.

Table 1: Physico-chemical properties for thiram (Van de Plassche, 1994)

MW	K_{aw}	$\log K_{ow}$	Kp_{soil}	$Kp_{sediment}$	k_{deg}	Readily biodegradable	Vp
240.44	-	1.76	24.5	24.5	-	-	-

MW = molecular weight (in g/mol)

K_{aw} = air-water partition coefficient

K_{ow} = octanol-water partition coefficient

Kp = partition coefficient (in l/kg)

k_{deg} = degradation rate constant in air (in $10^{-6}/s$)

Vp = vapour pressure (in kPa)

The partition coefficients (Kps) for soil and sediment are equal. The partition coefficient is calculated from the K_{ow} value using formula 22 (Van de Plassche, 1994).

2.2 Ecotoxicity data

Surface water

Toxicity data are only available on freshwater organisms; acute data on bacteria, algae, crustaceans, fish and amphibia and chronic data on green algae, crustaceans and fish (part III; appendix D). The lowest NOEC value is 0.32 $\mu g/l$ for fish (Van de Plassche, 1994).

Soil/sediment

Only chronic toxicity data are available on organisms exposed via contaminated soil (bacteria, fungi, microbial processes and enzyme activity) (part III; appendix D). The lowest NOEC value is 0.38 mg/kg for enzyme activity (Van de Plassche, 1994).

No toxicity data are available on organisms exposed via contaminated sediment (Van de Plassche, 1994).

Air

There are no (eco)toxicological data to derive an MPC in air.

Secondary poisoning

Two NOECs are available for birds while only one is present for mammals, showing a comparable toxicity (part III; appendix D). The lowest NOEC is 2.9 mg/kg food for birds (Van de Plassche, 1994).

No data on experimental BCFs are available. The calculated BCF for fish (formula 10) is 2.8 l/kg, while the one for bivalves (formula 11) is 0.7 l/kg. For earthworms a mean BCF of 1 l/kg (with a maximum BCF of 10 l/kg) is assumed (Van de Plassche, 1994).

2.3 (Human) toxicity data

No MPC_{human} has been derived yet.

3. Derivation of MPCs and NCs for different compartments

3.1 Surface water

Direct effects

To derive an MPC based on direct effects the modified EPA method is used, applying a factor of 10 on the lowest NOEC. This MPC based on data for freshwater fish, is 0.032 µg/l (Van de Plassche, 1994).

Indirect effects

MPC, based on the combined data sets for birds and mammals and calculated with the modified EPA method, is 0.29 mg/kg food (Van de Plassche, 1994).

To calculate the MPC for secondary poisoning, the BCF for fish (the most critical route) is used. This MPC, based on the combined data set of birds and mammals, is 33 µg/l (Van de Plassche, 1994).

Final MPC

The MPC for secondary poisoning is higher than the MPC in water based on direct effects, indicating that there is probably no risk of secondary poisoning via the aquatic route. Thus, the final MPC for the aquatic environment is set at 0.032 µg/l (Van de Plassche, 1994). The NC in surface water is $3.2 \cdot 10^{-4}$ mg/kg (table 2).

3.2 Soil

Direct effects

To derive an MPC in soil based on direct effects, the modified EPA method is used, applying a factor of 10 on the lowest NOEC. This MPC is 0.038 mg/kg in standard soil (Van de Plassche, 1994).

Indirect effects

The MPC for secondary poisoning in the terrestrial food chain, based on the combined data set for birds and mammals and calculated with the modified EPA method (using the BCF for earthworms) is 0.067 mg/kg (Van de Plassche, 1994).

Final MPC

Since the MPC for secondary poisoning is slightly higher than the MPC in soil based on direct effects, there is probably no risk of secondary poisoning at a concentration equal to the MPC based on direct effects. Thus, the final MPC in soil is set at 0.038 mg/kg, the MPC based on direct effects (Van de Plassche, 1994). The NC in soil is $3.8 \cdot 10^{-4}$ mg/kg (table 2).

3.3 Sediment

No toxicity data are present for sediment-dwelling organisms. Therefore an MPC of $7.9 \cdot 10^{-4}$ mg/kg is calculated using the equilibrium partitioning method (formula 6) (Van de Plassche, 1994). The NC in sediment is $7.9 \cdot 10^{-5}$ mg/kg (table 2).

3.4 Air

No MPC in air has been derived yet. For an alternative method to derive a critical concentration in air and rainwater, see § 4.

3.5 Overview of MPCs and NCs

Table 2: Overview of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different compartments

	Surface water (µg/l)	Soil (mg/kg)	Sediment (mg/kg)	Air (µg/m³)
MPC	0.032	0.038	$7.9 \cdot 10^{-4}$	-
NC	$3.2 \cdot 10^{-4}$	$3.8 \cdot 10^{-4}$	$7.9 \cdot 10^{-5}$	-

4. Harmonization of MPCs and NCs

Because only MPCs for surface water, sediment and soil are available, the harmonization procedure is performed using the equilibrium partitioning method. For the harmonization of the MPC in surface water with the MPC in soil, the MPC in soil based on toxicity data is compared to the MPC in soil calculated by means of the equilibrium partitioning method (formula 7). The MPC calculated by equilibrium partitioning (i.e. $7.9 \cdot 10^{-4}$ mg/kg) is a factor of 40 lower than the MPC in soil, being 0.038 mg/kg (table 2). No terrestrial toxicity data are available for target species, although these data are available for aquatic organisms. On the other hand, enzyme activity is a relatively sensitive endpoint if data for thiram are compared with data for other pesticides. Therefore it is decided to set the harmonized MPC in soil at 0.038 mg/kg, based on effects on soil organisms (Van de Plassche, 1994).

For air, critical concentrations in air and rainwater have been calculated in such a way that the MPC in soil will not be exceeded. The critical concentrations in air and rainwater are $1.4 \mu\text{g}/\text{m}^3$ and $51 \mu\text{g}/\text{l}$, respectively (Ministry of VROM, 1997). In table 3 an overview of the MPCs, NCs and critical concentrations is given.

Table 4: Overview of Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and critical concentrations (CritConc) for different compartments

	Surface water ($\mu\text{g}/\text{l}$)	Soil (mg/kg)	Sediment (mg/kg)	Air ($\mu\text{g}/\text{m}^3$)
MPC	0.032	0.038	$7.9 \cdot 10^{-4}$	-
NC	$3.2 \cdot 10^{-4}$	$3.8 \cdot 10^{-4}$	$7.9 \cdot 10^{-6}$	-
CritConc	-	-	-	1.4 (air) 51 ¹⁾ (rainwater)

1) the unit of the CritConc in rainwater is $\mu\text{g}/\text{l}$

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