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**The incorporation of human toxicity criteria into
Integrated Environmental Quality Standards.**

Discussion report supportive to the development of a
harmonisation strategy.

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List of Abbreviations

| | |
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| BCF | BioConcentration Factor |
| CCa | Critical Concentration in air: the $C_{ss_{air}}$ which is in equilibrium with MPC_{soil} |
| CSOIL | Computer model to derive Soil Clean-up Intervention Values |
| $C_{ss_{air}}$ | Steady state concentration in air |
| EATDE | Estimated Average Total Daily Exposure |
| EUSES | European Union System for the Evaluation of Substances |
| Hc | Henry's law constant |
| IEQS | Integrated Environmental Quality Standard "IEQS" refers to reference values which are used in policy. In this report "IEQS" is usually used in a general way, mostly referring to the project name or the general concept. Occasionally it is used to refer to the political reference values. The latter may differ from scientific "limit values" such as MPC, MPR or NC. |
| IV | Intervention Value for soil clean-up |
| K_{ow} | Octanol-water partition coefficient |
| $K_{p_{soil}}$ | Partition coefficient of a substance between soil particles and soil water |
| MPC_{air} | Maximal Permissible Concentration in air; analogous: $soil$ or $water$ |
| MPR | Maximal Permissible Risk level, usually determined after oral exposure of animals to substances. For substances with threshold effect this is equal to the TDI, for genotoxic carcinogens this is equal to the dose associated with an additional cancer risk of 1 per 10^4 life-time exposed people. The MPR is used as a measure for internal exposure as well, assuming 100% bioavailability after oral exposure and 75% bioavailability after inhalatory exposure. |
| NC | Negligible Concentration (usually defined as $MPC/100$) |
| PAH | Polycyclic Aromatic Hydrocarbon |
| PEC | Predicted Environmental Concentration |
| QSAR | Quantitative Structure-Activity Relationship |
| ECOTOX SCC | Ecotoxicological Serious soil Contamination Concentration |
| HUM-TOX SCC | human toxicological Serious soil Contamination Concentration |
| Sol | Solubility in water |
| TDI | Tolerable Daily Intake |
| USES | Uniform System for the Evaluation of Substances (previous version of EUSES) |
| Vp | Vapour pressure |

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Summary

This report has been prepared in the framework of the project "Setting Integrated Environmental Quality Standards" (IEQS-project). The aim of the project is to derive Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for substances for the different environmental compartments: air, water, sediment and soil. The risk limits which have been derived up to now can be characterised by two principal properties:

1. they provide an accepted level of safety for ecosystems and in some cases for humans,
and
2. the risk limit in one environmental compartment will not be exceeded when the risk limit in another compartment is reached, due to inter-compartmental exchange.

In previous reports MPCs and NCs were derived for metals, polycyclic aromatic hydrocarbons (PAHs) and various (volatile) organic substances, based on ecotoxicological data. Although inter-compartmental harmonisation (second characteristic) was achieved, incorporation of human toxicological criteria (first characteristic) has not been accomplished to a large scale up to now. For PAHs and metals it was assumed that ecosystems and in much lesser extent, humans would be exposed via water, sediment and soil. Only for volatile organic substances a first attempt has been made to incorporate human toxicological criteria, assuming that for these substances inhalation is the predominant route of exposure for humans, and that humans are the most sensitive protection goal.

The aim of the present report is to evaluate whether the ecotoxicologically derived MPCs from the IEQS-project, sufficiently protect humans, for (volatile) organic substances, PAHs and metals. The results of this study are meant to provide input for the discussion on how to deal with humans as a protection goal within the IEQS-project.

Estimates of human multi-route exposure patterns are calculated with the computer programme EUSES 1.0. The concentration of the substances in the different environmental compartments were set at the respective MTR. The total daily exposure for humans is calculated using EUSES, and is compared to relevant human toxicological criteria.

The major findings of the study are that:

1. for the compounds studied only for (volatile) organic substances sufficient data were available to calculate multi-route exposure patterns and estimates of total daily exposure.
For PAHs the comparison between total daily exposure and human toxicity criteria could not be made because the toxicological criteria for the individual substances were lacking.
For metals estimates of total daily exposure could not be calculated because of insufficient data and/or inappropriate models,

2. for many volatile substances, it cannot be excluded that human toxicological criteria may be exceeded if environmental concentrations are maintained at (ecotoxicological) MPC levels, and
3. for many volatile substances, environmental concentrations maintained at the environmental risk limits may result in exposure patterns for humans in which other routes than inhalation are of predominant importance.

Since for PAHs and metals, either the EUSES calculations or their interpretation was limited, Intervention values (IV-values) for soil remediation were evaluated as well. The IV-values are selected from the lowest of the two values from ecotoxicological and human toxicological criteria.

For 40% of the (volatile) organic substances, for the metals and for the PAHs, the IV-values are based on ecotoxicological criteria, while for the remaining (volatile) organic substances, the IV-values are based on human toxicological criteria. These differences may be caused by humans being more sensitive than ecosystems or vice versa, differences in the availability of data, the use of different uncertainty factors, etc.

It is concluded that integration of both ecotoxicological and human toxicological information is required to derive harmonised environmental quality standards which display the characteristics as mentioned earlier. Moreover, focusing at only one possible route of human exposure is considered an approach, too limited. Even for very volatile substances other routes than inhalation may significantly contribute to the total exposure.

From the results of the report the following discussion points can be distilled for the discussion on how to deal with humans as a protection goal within the IEQS-project.

- whether ecotoxicological and human toxicological information is to be included in deriving environmental risk limits or quality standards;
- for which substances is there a need to include ecotoxicological and human toxicological information in deriving environmental risk limits or quality standards (for example, must a multi-route exposure model be used for volatile substances);
- for which environmental risk limits or quality standards is there a need to include ecotoxicological and human toxicological information;
- whether EUSES is a suitable and realistic multi-route exposure model for humans;
- whether there is a need for a further analysis of the parameters that are used in the models (EUSES and CSOIL).

When ecotoxicological and human toxicological criteria are integrated for deriving risk limits, the EUSES programme can be used to calculate sets of environmental concentrations that are maximised either with respect to the most sensitive compartment, i.e. the compartment in which the MPC is reached first, or with respect to the MPC for humans.

Samenvatting

Dit rapport is opgesteld in het kader van het project “Integrale Normstelling Stoffen” (INS-project). Dit project beoogt Maximaal Toelaatbaar Risiconiveaus (MTRs) en Verwaarloosbaar Risiconiveaus (VRs) voor stoffen af te leiden voor de afzonderlijke milieucompartimenten: lucht, water, sediment en bodem. Vooral nog kunnen twee hoofdkenmerken van dergelijke risiconiveaus worden onderscheiden:

1. zij voorzien in een geaccepteerd niveau van veiligheid, namelijk voor ecosystemen en in sommige gevallen voor de mens en
2. handhaving van het risiconiveau in het ene milieucompartiment leidt niet tot overschrijding van het risiconiveau in een ander compartiment als gevolg van intercompartimentale uitwisseling.

In vorige rapportages werden MTRs en VRs afgeleid voor metalen, polycyclische aromatische koolwaterstoffen (PAKs) en diverse (vluchtige) organische verbindingen, gebaseerd op ecotoxicologische gegevens. Hoewel intercompartimentale harmonisatie (tweede eigenschap) is gebeurd, is afstemming met humaan-toxicologische criteria (eerste eigenschap) tot nu toe nog niet op grote schaal gerealiseerd. Bij PAKs en metalen is verondersteld dat met name het ecosysteem en in mindere mate de mens zou worden blootgesteld via water, bodem en sediment. Slechts voor de vluchtige stoffen is een eerste poging gewaagd om tot zo'n afstemming te komen, onder de aanname dat voor de mens inhalatie de meest belangrijkste route van blootstelling is voor dergelijke stoffen en de mens het meest gevoelige beschermingsdoel is.

Het doel van het voorliggende rapport is na te gaan of de in het INS-project ecotoxicologisch onderbouwde MTRs voldoende bescherming bieden voor de mens voor (vluchtige) organische verbindingen, PAKs en metalen. De resultaten van dit onderzoek zijn bedoeld ter ondersteuning van de te voeren discussie hoe om te gaan met de mens als beschermingsdoel binnen het INS-project.

Er zijn schattingen gedaan van multi-route blootstelling voor de mens, berekend met het computer programma EUSES 1.0. Hiertoe is de concentratie van de verschillende onderzochte stoffen in de diverse milieucompartimenten gesteld op het niveau van de MTR. Met behulp van EUSES is berekend wat de totale dagelijkse blootstelling is voor de mens, die is vergeleken met de relevante humaan-toxicologische criteria.

De belangrijkste bevindingen van de studie zijn dat:

1. van de onderzochte verbindingen alleen voor (vluchtige) organische stoffen voldoende gegevens beschikbaar zijn om multi-route blootstellingspatronen en schattingen van de totale dagelijkse blootstelling van de mens te berekenen. Voor PAKs kon de vergelijking tussen de totale dagelijkse blootstelling mens en de humaan-toxicologische criteria niet worden gemaakt, omdat voor individuele stoffen geen toxiciteitscriteria voor de mens zijn afgeleid. Voor metalen konden geen schattingen van de humane blootstelling worden berekend, omdat er te weinig gegevens beschikbaar waren, of omdat de mathematische modellen niet zijn toegesneden om zo'n schatting te kunnen maken;

2. voor vele vluchtige stoffen kan niet worden uitgesloten dat concentraties in het milieu, die worden gehandhaafd op het niveau van de (ecotoxicologische) MTR, kunnen resulteren in een overschrijding van de humaan-toxicologische criteria en
3. voor vele vluchtige stoffen blootstellingspatronen voor de mens worden berekend, waarin ook andere blootstellingsroutes dan via inhalatie belangrijk zijn.

Omdat voor PAKs en metalen de EUSES-berekeningen of de interpretatie ervan problemen opleverden, werd tevens een inventarisatie van interventiewaarden (IV-waarden) opgenomen. Bij de afleiding van de IV-waarden is namelijk een afstemming van ecotoxicologische met humaan-toxicologische criteria aan de orde. De IV-waarden worden vastgesteld op basis van de meest strenge waarde uit ecotoxicologische- en humaan-toxicologische informatie.

Voor 40% van de (vluchtige) organische verbindingen, voor de metalen en voor de PAKs blijken de ecotoxicologische criteria het laagst te zijn bij de bepaling van de IV-waarden. Voor de overige (vluchtige) organische verbindingen blijken de humaan-toxicologische criteria het laagst te zijn. Dit kan meerdere oorzaken hebben, namelijk een hogere gevoeligheid van de mens voor de verbinding of vice versa, een verschil in beschikbaarheid aan gegevens voor mens en ecosysteem, een verschil in veiligheidsfactoren, etc.

Er wordt geconcludeerd dat integratie van zowel ecotoxicologisch als humaan-toxicologische informatie een vereiste is om tot risiconiveaus te komen die beide eerdergenoemde eigenschappen hebben. Tegelijkertijd blijkt dat een benadering waarin slechts één blootstellingsroute (inhalatie) wordt betrokken te beperkt van opzet is. Zelfs voor zeer vluchtige stoffen kunnen andere routes dan blootstelling via inhalatie in aanzienlijke mate bijdragen aan de totale blootstelling van de mens.

Uit de resultaten van het rapport kunnen de volgende discussiepunten worden gedistilleerd die van belang zijn voor de te voeren discussie hoe om te gaan met de mens als beschermingsdoel binnen het INS-project.

- of ecotoxicologische én humaan-toxicologische informatie dient te worden meegenomen voor het afleiden van risiconiveaus of normen;
- voor welke stoffen behoefte is aan het meenemen van ecotoxicologische én humaan-toxicologische informatie voor het afleiden van risiconiveaus of normen (dient er bijvoorbeeld ook voor vluchtige verbindingen een multi-route blootstelling te worden meegenomen);
- voor welke risiconiveaus of normen behoefte is aan het meenemen van ecotoxicologische én humaan-toxicologische informatie;
- of EUSES een geschikt realistisch multi-route blootstellingsmodel voor de mens is;
- of er een nadere analyse nodig is van de parameters die in de modellen (EUSES en CSOIL) worden gebruikt.

Als humaan- en ecotoxicologische informatie geïntegreerd wordt voor de afleiding van risiconiveaus, kan het EUSES programma worden aangewend om stelsels van concentraties in het milieu te vinden, die ofwel gemaximaliseerd zijn met betrekking tot het compartiment, waarin de MTR het eerst wordt bereikt, ofwel gemaximaliseerd zijn met betrekking tot de MTR voor de mens.

1. Introduction

1.1 General aspects

This report is produced in the context of the project "Setting Integrated Environmental Quality Standards". This project started in 1989 as a result of the actions proposed in the National Environmental Policy Plan [1]. The aim of the project is to derive concentration limits for substances in the environment for the different compartments, air, water, sediment and soil. The project finds its political background in the risk philosophy of the Dutch Ministry of Housing, Spatial Planning and the Environment (Ministry of VROM) and is laid down in the document "Premises for Risk Management" [2]. These concentration limits are referred to as Integrated Environmental Quality Standards (IEQSs) in Dutch environmental policy.

The IEQSs set by the Ministry of VROM are based on risk limits, the Maximum Permissible Concentration (MPC) and Negligible Concentration (NC). The MPC for the different compartments is derived using (eco)toxicological data and represents the potential (eco)toxicological risk of the substance in question. The NC is obtained by dividing the MPC by 100, taking into account simultaneous exposure to a variety of substances. Derivation of MPCs and NCs is performed at the National Institute of Public Health and the Environment (RIVM¹).

The ecotoxicologically based MPC aims at the protection ecosystems via protection of all wildlife species. For practical purposes and in order to be able to use statistical extrapolation methods like the one of Aldenberg and Slob [3], a 95% protection level is chosen as a cut-off value [2]. The concentration corresponding to a 95% protection level is called the MPC and can be derived using statistical extrapolation methods if chronic ecotoxicity data for more than four taxonomic groups are available. Alternatively, if less chronic or only acute ecotoxicity data are available, the preliminary effect assessment or modified EPA-method is applied in which uncertainty factors are used.

For the protection of humans the criteria aim at protection of the individual. Environmental concentrations must be so low that humans are not exposed above a Maximum Permissible Risk (MPR) level which is equal to the TDI (Tolerable Daily Intake) for substances eliciting threshold effects. For genotoxic carcinogens (no threshold assumed) the MPR is the dose associated with an additional cancer risk of 1 per 10⁴ life-time exposed people [2].

One of the requirements of the IEQSs is that they are harmonised, meaning that when the concentration of a particular contaminant in an environmental compartment reaches the IEQS-level for that contaminant in that compartment (e.g. air or water), this does not lead to unacceptably high concentrations of that contaminant in the other compartments. In addition the various IEQSs have to guarantee that for environmental organisms as well as for human beings the accepted level of safety will not be exceeded. Therefore, to derive IEQSs for individual substances both ecotoxicological and human toxicological data, e.g. MPCs, and MPRs have to be taken into account.

¹ Abbreviation in Dutch for "National Institute of Public Health and the Environment"

For aquatic organisms, exposure to environmental contaminants is mainly through one contact medium (i.e. water) although the source of the contaminant may originate in other media. For fish, for example, exchange processes such as deposition from air or leaching from soil may contribute to the contaminant's concentration in the water. Therefore, MPCs for aquatic organisms are fairly simple to derive from aquatic toxicity data.

For humans the situation is more complex. While air is a direct exposure medium for humans, contact with unpurified water is limited to swimming because drinking water is usually purified before it is distributed. Nevertheless, people can be exposed to chemicals in drinking water. Direct contact with soil and thus soil contaminants is limited too, usually to ingestion of soil by children and to ingestion of soil residues on vegetables. Additionally, uptake of chemicals by humans may take place through the food chain, because both plants as well as animals used for human consumption are exposed to environmental contaminants. Thus, for humans more routes of exposure are of relevance than e.g. for a fish. Therefore derivation of MPCs based on human toxicity data for water and soil is very difficult because of the indirect nature of the exposure. Derivation of a human MPC for air may be less complex. This is particularly so if it is assumed that for certain substances inhalation is the predominant route of exposure. This may for instance be the case for chemicals with a high vapour pressure or a high air-water partition coefficient.

A similar complex exposure situation can be recognised for mammals and birds. Estimation of exposure for these groups of animals is, however, beyond the scope of the present document and has been treated in a series of RIVM reports on risk of secondary poisoning [4].

1.2 Progress up to now

Until now harmonisation of MPCs has been performed, firstly by applying the equilibrium partitioning method to ensure that MPC for water and soil are harmonised. Secondly, by applying the computer model SimpleBox to ensure that MPC_{eco} s for water and soil are harmonised with human risk levels (Van de Meent, 1993; Van de Plassche *et al.*, 1993) and assuming that exposure of humans is mainly through air. In principle, when the harmonisation results in a lower value than the MPC proposed for a certain compartment, the MPC_{eco} s were adjusted (see fig 1).

This is worked out below in more detail:

- I. For a number of volatile substances Maximum Permissible Concentrations in air ($MPC_{air, human}$) have been derived [5, 6], while ecotoxicologically based MPC_{air} are highly speculative, if available at all [7]. Therefore, in subsequent studies the $MPC_{air, human}$ s have been harmonised with ecotoxicologically based Maximum Permissible Concentrations in soil and water ($MPC_{soil, eco}$, $MPC_{water, eco}$; cf. ref. 3). For this harmonisation it was assumed that:

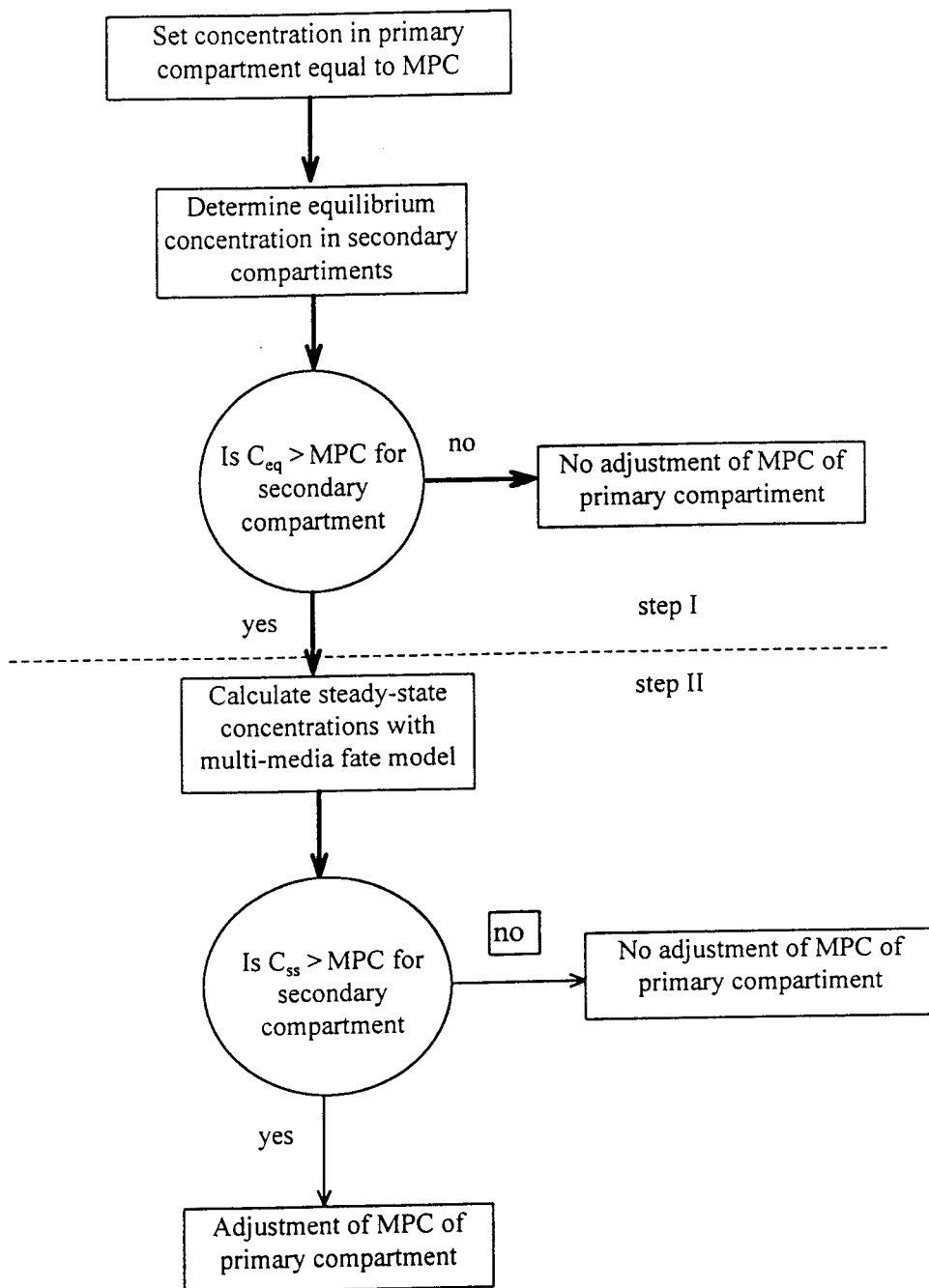


Figure 1. Two step procedure as followed by Van de Plassche and Bockting [5] for the harmonisation of MPCs for volatile substances. Emissions of environmental contaminants are allocated to the primary compartment. The secondary compartments receive the contaminants through redistribution from the primary compartment. In the first step (above the dotted line) calculations are based on equilibrium partitioning (C_{eq}). In the second step using the SimpleBox Model, steady state concentrations (C_{ss}) are calculated.

- A. for humans inhalation is the predominant route of exposure for volatile substances, and
- B. $MPC_{soil, eco}$ and $MPC_{water, eco}$ need only be adjusted (read: decreased) if at these concentrations the accepted human-toxicological risk level for air is exceeded, or, in other words, if the steady state concentration in air ($C_{ss, air}$) which is compatible with the $MPC_{soil, eco}$ and $MPC_{water, eco}$ is greater than the $MPC_{air, human}$.

The (preliminary) harmonisation procedure was carried out in two steps (fig. 1):

In the initial step it was demonstrated that if for these volatile substances primary emission to air was assumed, maintenance of the limit value or (preliminary) $MPC_{air, human}$ would not result in the MPC_{eco} s (i.e. MPCs for soil, water and sediment) to be exceeded.

In the second step steady state calculations were carried out using the Mackay level III-type model "SimpleBox" [8], under the assumption that the primary compartment to which emission occurs was water. Under this assumption it was demonstrated that if steady state concentrations were equal to the $MPC_{water, eco}$ it could not be excluded that for a number of these substances the $C_{ss, air}$ might exceed the $MPC_{air, human}$.

Depending on the quality of the data and the ratio between the expected (calculated) $C_{ss, air}$ and $MPC_{air, human}$, the MPCs for water, soil and sediment were adjusted downwards [7]. In the adjustment procedure the reliability of the predicted $C_{ss, air}$ was taken into account. This reliability was estimated in a sensitivity analysis of SimpleBox in which the influence of variations in lipophilicity, volatility and photo-degradation rate in air was studied [7, 9]. In the report by Van de Plassche and Bockting [7] this uncertainty was estimated to amount to a factor of 10. More recently Etienne *et al* [9] have shown that this uncertainty may be considerably less².

In the end, only for benzene, 1,2-dichloroethane, 1,2-dichloropropane, trichloromethane and vinylchloride the MPCs for water, soil and sediment needed to be adjusted downwards with factors of 10, 20, 70, 10 and 10, respectively [7]. The MPCs for the other substances were not adjusted. The reasons for this were either too small a ratio between $C_{ss, air}$ and $MPC_{air, human}$ (ratio less than 10; 13 chemicals), or the availability of only a preliminary $MPC_{air, human}$ (21 chemicals) or unavailability of an $MPC_{air, human}$ (6 chemicals).

For volatile substances the assumption of primary emission to the water compartment is not entirely realistic [7]. It has been demonstrated that these substances are largely emitted to air. However, because for none of these substances emission to water could be excluded, the assumption was

² The uncertainty factor of 10, as estimated by Van de Plassche and Bockting [7], was used to determine adjustment factors for 18 substances. This new evaluation by Etienne *et al* [9] may necessitate a re-evaluation of the data of Van de Plassche and Bockting [7].

considered valid with respect to the main issue of the study: determination of compatibility of MPCs for the various compartments. A more extensive description of the procedure can be found in Van de Plassche and Bocking [7].

II. In a pre-study to the present one, Mennes *et al.* [10] have calculated human multi-route exposure patterns for five substances of different (physico)-chemical nature, namely atrazin, 1,4-dichlorobenzene, benzene, benzo(a)pyrene and dichloromethane. For these calculations the risk assessment model USES 1.0 [11] was used. This computer model consists of several modules. The most relevant modules in the context of the present study are:

1. an emission module, in which emission patterns are determined, based on substance characteristics, quantities produced or used, industrial category and life cycle step under study.
2. a distribution module, which is very similar to (and derived from) the SimpleBox model. In this module dynamic steady state concentrations are computed, for air, agricultural, natural and industrial soil, soil pore water and surface water
3. a human intake module, in which concentrations of environmental contaminants in human contact materials (air, drinking water, food) is determined and the average multi-route exposure of humans is estimated.

The default approach via which emission patterns are determined was circumvented as much as possible by feeding the model with realistic emission data. By comparison of the exposure patterns generated by the model with actual exposure data, it was shown that the USES 1.0 model provided a fairly realistic insight in the relevance of various routes of exposure (i.e. air, water and food) [10].

The results demonstrated that at a regional scale drinking water and consumption of leaf- and root crops were the major routes of exposure for atrazin, while for benzo(a)pyrene leaf crops were the most important. For all three volatile substances (1,4-dichlorobenzene, benzene and dichloromethane) it was shown that inhalatory exposure was by far the most important route. Thus from this study [10] it was concluded that, assumption I.A (inhalatory exposure is most relevant for volatile substances) is confirmed by the model calculations, at least if these are based on realistic emission patterns.

III. The integration of human- and ecological limit values is also an aspect of the procedure via which proposals for Intervention Values for soil clean-up (IV) are derived. Up to now for 126 substances [12,13,14,15] such proposals for IVs have been derived.

The Intervention Values are founded on the ecotoxicological criterion ECOTOX SCC (ecotoxicological Serious soil Contamination Concentration) and the human toxicological criterion HUM-TOX SCC (human toxicological

Serious soil Contamination Concentration) [14,16]. Basically, integration of the HUM-TOX SCC with the ECOTOX SCC is choosing between the lowest of the two. In addition, in this choice the reliability of the underlying toxicological data set is taken into account. Other aspects taken into account when deriving a final Intervention Value for soil clean-up are permissible concentrations in drinking water and the natural background (e.g. for metals) [14,17]. Some more details on the procedure are given in chapter 2, section 2.1.

It must be noted that in the derivation of Intervention Values human toxicological criteria (MPRs and MPCs) are incorporated, among other criteria. The human toxicological criteria are generally applicable in any toxicological risk assessment and are not specifically derived to protect humans in case of a local soil contamination situation.

When Intervention Values are exceeded the location is recognized as a site of serious soil contamination. Further investigation (e.g. with respect to exposure and risk, or present or expected use of the site) must indicate whether remediation has to be carried out immediately or can be postponed³.

1.3 Goal of the present report

The present report has been written to support the further development of a method to integrate ecotoxicologically-based MPCs for (air), water, soil and sediment with human toxicological criteria, in particular $MPC_{air, human}$ and MPR. Given the MPC_{ecoS} and MPC_{airS} which have been derived previously, the question arises whether these MPCs provide sufficient protection for humans. In order to gain insight into this matter human exposure to individual substances will be estimated with a computer model, using the MPCs for the various compartments as starting points.

Therefore:

1. A short overview of the results from the IV-project will be presented. It is anticipated that the results in the IV-framework may give a first indication of the relevance of MPC_{ecoS} versus $MPC_{air, humanS}$ or MPRs in the process of developing IEQs when these risk limits are weighed against each other.
2. An inventory of the data which are available for the volatile substances as indicated above will be presented. In addition, for a number of metals and polycyclic aromatic hydrocarbons (PAHs) sets of ecotoxicological MPCs have been derived, recently. Based on these data it will be decided whether a meaningful estimation of human multi-route exposure can be calculated. For substances for which a meaningful estimation of human exposure is not possible, the inventory may indicate for which substances additional data have to be generated. Meaningful in this context should be interpreted as “can be compared with a human toxicological criterion” or “has sufficient reliability”

³ A more elaborate description of the term “Intervention Values” can be found in ref 15.

3. Finally, confirmation is wanted whether the currently available IEQs (see ref. 7) are compatible with previously derived MPRs (Maximal Permissible Risk level), for human toxicity. This question seems to be of importance in particular for some less volatile substances which have been treated previously as if they were volatile (e.g. tetra- and penta and hexachlorobenzene; see ref. 7).

Estimates of human multi-route exposure will be calculated and subsequently be compared to the MPRs. Based on the outcome of these calculations decisions can be made as to the background assumptions, choices and uncertainties, aiming at a further refined methodology to derive both ecotoxicologically and human toxicologically based Integrated Environmental Quality Standards.

1.4 Substances

The substances which are considered in the present report are listed in the various tables in appendix I. Among these substances are a number of metals, PAHs and volatile organic substances, of the so called 2-b list [18]. MPC_{ecoS} , $MPC_{air, human}$ and MPRs have been published in several earlier reports by RIVM.

2. The project “Intervention Values for soil clean-up”

It was anticipated that for PAHs and metals calculations with EUSES would be either impossible or difficult to interpret. This would obstruct the evaluation of the available MPC_{eco} for these substances with respect to their “safety” for humans as mentioned in paragraph 1.3. However, as mentioned before, a similar weighing of ecotoxicological and human toxicological information is carried out within the Intervention Values project. One might expect that if for a particular substance the Intervention Value is based on ecotoxicological criteria instead of human toxicological criteria (i.e. ecosystems are more sensitive than humans), it would be possible to extrapolate this finding to the IEQS-project, thus leaving the human toxicological criteria out of consideration and assuming extensive calculations with EUSES for PAHs and metals to be unnecessary.

Therefore, this chapter gives some information on the methodology followed in the IV project and on its results. These results will be further discussed in chapters 5 and 6.

2.1 a short introduction on the methodology

The first step in the derivation of Intervention Values is the determination of concentrations or exposure levels above which the environment or human beings may be seriously at risk. The ecotoxicological criterion is called the ECOTOX SCC: the ecotoxicological Serious soil Contamination Concentration, which is the concentration in soil or groundwater at which 50% of the species and 50% of the microbial processes are protected⁴ [14,16].

The human toxicological criterion is called HUM-TOX SCC: the human toxicological Serious soil Contamination Concentration. This concentration is derived from the MPR. In order to derive the HUM-TOX SCC from the MPR, the CSOIL model [12] is used to generate estimates of human multi-route exposure at different concentrations of the chemical in the soil. The concentration of the chemical in the soil at which the MPR is reached is the HUM-TOX SCC.

For determination of the human exposure pattern the following routes are taken into account:

- dermal contact with soil contaminants
- inhalation of contaminated soil particles
- inhalation of vapours of contaminants in the drinking water while taking a shower
- outdoor and indoor inhalation of vapours
- ingestion of contaminated soil
- ingestion of contaminants via consumption of locally grown vegetables
- ingestion of soil contaminants via drinking water

For calculation of the multi-route exposure with CSOIL, it is further assumed that contamination of drinking water only occurs at the site of the contamination because of permeation of substances through the water mains or, in other words: the drinking water leaving the purification plant is essentially free of contaminants. Furthermore,

⁴ This is a difference with the IEQS-programme in which the ecotoxicological criterion $MPC_{eco, soil}$ is used, The $MPC_{eco, soil}$ is the concentration at which 95% of the species is protected [7]. The ECOTOX SCC (aiming at 50% protection) is thus less stringent than the $MPC_{eco, soil}$.

intake via consumption of animal products is not an element in the exposure assessment for local soil contamination scenarios, because it is assumed that fish, dairy products and meat are purchased elsewhere.

Subsequently, the result of the CSOIL computations (= HUM-TOX SCC) is put to test to see if it is compatible with e.g. MPC_{air}, permissible levels for plants (residues) or olfactory thresholds [12]. Incompatibility may lead to downward adjustment of the HUM-TOX SCC.

Finally, the Intervention Value is chosen as the being lowest of either HUM-TOX SCC or ECOTOX SCC. In this choice the reliability of the underlying toxicological data set is taken into account.[16,17,15,19].

2.2 a short discussion of the results

A list of HUM-TOX SCC, ECOTOX SCC and Intervention Values is presented in appendix II. This list is limited with respect to the number of substances: only those which are incorporated in the present report (i.e. the IEQS-project) are mentioned. The data in this appendix have been taken from ref. [19], in which final values have been given for the first 80 substances for which IVs were derived. Data for the remaining substances were taken from refs. [13], [14] and [15].

From the list it can be seen that the Intervention Values of 22 of the 27 volatile substances of the IEQS project, are based on the HUM-TOX SCC, while for the metals (except Sb and Tl) and PAHs the ECOTOX SCC is the most stringent criterion. Thus it is conceivable that harmonisation of eco- with human toxicological criteria may be equally important for at least part of the substances.

From the underlying reports [12,14,15,16] it can further be concluded that, following the lines of the CSOIL model, for human exposure to soil contaminants three routes are the most prominent ones: intake via ingestion of soil, intake via consumption of home-grown vegetables and intake via indoor inhalation of vapours. This is shown in the following list (after ref. 12):

| type of substance: | soil ingestion | plant consumption | indoor inhalation | comment |
|-------------------------------------|----------------|-------------------|-------------------|--|
| metals | 8 - 53% | 47 - 92 % | | |
| anions | | 100% | | e.g. PO ₄ ³⁻ , Br ⁻ , CN ⁻ , S ²⁻ |
| PAHs | 3 - 85 | 6 - 93% | | excl. naphthalene |
| very volatile ⁵ organics | | 0 - 65% | 19 - 100% | e.g. benzene, fenol, toluene, (chlorinated) alkanes |
| less volatile organics | | 0 - 17% | 82 - 100% | higher chlorinated aromatics and cycloalkanes |
| “non-volatile” organics | 12 - 84% | | 5 - 86% | e.g. DDT, drins, phthalate, maneb |

⁵ In this table “volatile” refers to vapour pressure. For environmental distribution of substances air/water- and air/soil-partition coefficients are also important.

For metals, various anions (e.g. Br⁻, F⁻, CN⁻; not in the IEQS-project) and for PAHs intake via ingestion of soil and consumption of locally grown vegetables are the most prominent routes. Exposure via inhalation of contaminated indoor air is of varying importance for other (volatile) organic chemicals. The exposure to contaminants via inhalation of soil particles or via inhalation vapours while taking a shower is unimportant. Contact via drinking of water was only relevant for cresol (13%), while intake via direct contact of soil with skin was only relevant for the PAHs and maneb (max. 10%).

3. Methodology

Two main purposes of this report are 1) collection of data needed and 2) estimation of human multi-route exposure. Conceivably the type of the data to be collected depends on the methodology via which human multi-route exposure will be estimated. Therefore, in this chapter a short introduction to this methodology will be presented. In addition, some attention is paid to criteria and sources used for data collection.

3.1 Estimation of human multi-route exposure and health risk

3.1.1 starting points

For the estimation of human multi-route exposure the appropriate modules in the risk assessment model EUSES 1.0 [20] will be applied. In these modules human food, air and drinking water consumption are basic data to estimate intake through the various exposure routes.

For each substance the starting point in this exposure assessment is the set of either harmonised or preliminary MPCs as described in earlier reports [7, 21, 22]. These MPCs are entered into the EUSES model as regional PECs, assuming that the MPC_{water} is representative for soil (pore-) as well as surface water and that the MPC_{soil} is representative for both natural and agricultural soil. The concentration in air will be set equal to $MPC_{\text{air, human}}$. The PEC in industrial soil is set at 0 mg/kg, assuming that contamination of industrial soil is local and that exposure of the general population to contaminated industrial soil is negligible. It must be noted that this procedure reduces the EUSES model to its very final steps: i.e. only calculations which are of immediate relevance to human exposure were used. These include:

Exposure (intake) via drinking water:

The intake via drinking water is calculated as the product of daily water consumption and concentration in drinking water. EUSES follows a worst-case approach in which the concentration of a substance in drinking water is equal to the highest concentration in either purified surface water or groundwater. For groundwater, which is the pore water under agricultural soil, no effective purification is assumed. As in the approach described above surface and groundwater have equal concentrations, purification is irrelevant: the concentration of a substance in drinking water will always be equal to the $MPC_{\text{water, eco}}$. For a number of substances the effect of this approach will be studied in a second scenario in which the groundwater concentration is set at 0 mg/l; which forces EUSES to use the concentration in purified surface water as the concentration in drinking water.

Exposure (intake) via consumption of fish:

which is calculated from the concentration of the substance in surface water, the bioconcentration in fish (estimated from K_{ow}) and the average daily consumption of fish⁶.

⁶ Because this model is K_{ow} -driven, it does not directly apply to metals

Exposure (intake) via consumption of leaf and root crops:

which is calculated from the concentration of the substance in pore water in agricultural soil and from the concentration in air. Factors influencing the concentration in the plant tissues are uptake from soil by roots and transport from roots to leaves, growth rate, biotransformation in plant tissues, photolysis and equilibrium partitioning between leaves and air. Aerosol deposition is no part of the model. For root crops the concentration of the substance in the plant tissues is directly calculated from its concentration in pore water and the K_{ow} ⁶

Exposure via consumption of milk and meat products:

which is calculated from the average human daily intake of these animal products and the contaminant concentrations in them. The concentrations of the substance in these products are calculated from the daily intake of the chemical by cattle, multiplied by bioaccumulation factors. The latter are estimated from the K_{ow} . The daily intake of a substance by cattle is calculated from the intake via grass (\approx leaf crops), soil, air and drinking water⁶.

Exposure via air:

which is calculated from the inhalable concentration in air and the daily amount of inhaled air.

Exposure via the skin:

For environmental contaminants, dermal exposure is not incorporated in the EUSES model.

For further details the reader is referred to the extensive description of EUSES [20]

3.1.2 adaptation of the EUSES model to the Dutch situation

Because EUSES 1.0 has been developed to serve European policy making, the default human consumption rates in EUSES 1.0 reflect the highest country-average consumption rates of all EU member states, in accordance with the Technical Guidance Document [20,23]. However, for the present research the EUSES defaults have been adapted to accommodate the Dutch situation, because its results are intended to support Dutch legislation. Therefore, the default consumption rates used were adapted and taken from the USES 1.0 model [11] (which is designed to model the Dutch situation) and have been presented in appendix III. In general these USES defaults will result in lower estimates of total daily exposure. The relative contribution via air and dairy product will become higher, while intake via root and leaf crops, and fish will become less important. Relative exposure via consumption of meat products is about equally important for the “Standard Dutchman” as it is for the “Standard European”.

3.1.3 soil ingestion

The EUSES programme does not take into account the exposure resulting from the ingestion of contaminated soil. Although for volatile substances soil ingestion does not seem to be an important route of exposure, for less volatile substances this may contribute to the total exposure to quite a considerable extent [12]. Therefore in this project soil contamination will be incorporated. This route, additional to the EUSES programme was quantified separately from EUSES calculations, using a simple Microsoft EXCEL spreadsheet. The following calculation, taken from the CSOIL model [12], was used to estimate human exposure to soil contaminants present at MPC_{soil} -level :

$$\text{Soil exposure } (\mu\text{g/kg b.w./d}) = C_{\text{soil}} \times \text{Soil ingestion} \times \text{bioavailability} \times 10^{-3} / \text{body weight.}$$

in which:

C_{soil} = the concentration of a contaminant in soil (in this case equal to MPC_{soil}) in mg/kg
 Soil ingestion = 50 mg per adult per day
 bioavailability = 1
 scaling factor = 10^{-3}
 body weight = 70 kg.

3.1.4 metals

The EUSES model was designed to assess the risks resulting from production, industrial manipulation and use of organic chemical substances. It is not directly suitable to calculate human exposure to metals, because the uptake-, bioaccumulation- (e.g. in plants, fish and cattle) and water purification-models are driven by the K_{ow} constant, which for metals is not very useful, because other processes are probably more relevant (i.e. active uptake mechanisms, see ref. 24). Plant uptake and bioaccumulation of metals in the human food chain can be estimated, though, using bioaccumulation factors, which have been determined in field or laboratory experiments. For exposure via drinking water, it will be assumed that metals which are present in soil or surface water will not be removed during purification, by setting the predicted concentration in drinking water equal to the MPC_{water, eco}.

3.1.5 physico-chemical constants

Evaluation with the EUSES model requires the availability of a minimum set of physico-chemical parameters i.e. octanol-water partition coefficient, molecular weight, solubility and vapour pressure [20]. Either such data or meaningful alternatives must be available. The latter is of relevance in particular in the case of metals. In previous reports (e.g. ref. 22) very extreme defaults were used to model environmental behaviour of metals.

3.1.6 relevance of the exposure estimates in terms of health risk

The intake via all routes is summed providing an estimate of the average total daily exposure (EATDE). This EATDE can be considered a measure for daily exposure or more precise, assuming 100% bioavailability after oral intake and 75% bioavailability after inhalatory exposure, a measure of daily systemic exposure, which can be

compared to the MPR. If the EATDE exceeds the MPR a risk for human health may be indicated.

It should, however, be noted that differences may exist between inhalatory and oral exposure. The severity or nature of the effects is not always similar for both routes of exposure. For instance, substances may be airway irritants or even carcinogenic after inhalatory exposure, while such effects are not observed after oral exposure. Thus decisions with respect to presence or absence of a human health risk should take into account this route specificity.

3.2 Data collection and data validation

Preferably, data will be taken from previous reports by RIVM. With respect to ecotoxicological MPCs, exclusively RIVM data are used because these values are already harmonised (requirement for the present project). Human health risk advisories (MPRs), physico-chemical and bioaccumulation data were also taken from earlier RIVM reports. If in an individual case no RIVM data were found, a value was taken from readily available literature sources, however, without any further validation. At any rate it was checked whether data met the input requirements of EUSES (e.g. dimensions, referring to wet weight, dry weight or fat content).

4. Availability of data and consequences of data gaps

The results of the survey into the availability of data have been listed in a number of tables which are presented in appendix I. In the following text these results are discussed. Substances are subdivided into three groups: volatile organic substances, PAHs and metals. The group of volatile substances will be treated first, because for this group some work on integration of human and ecotoxicological criteria ($MPC_{air, human}$ and MPC_{eco}) has been done already [7]. Next, the PAHs and metals will be discussed. Finally, the results of the data survey will be discussed and a decision will be presented for which substances further evaluation will be carried out.

4.1 Available data for the three groups of substances

4.1.1 volatile organic substances

From the original list (see ref. 18) two substances (xylene-mix and hexachloro-butadiene) were not further discussed by Van de Plassche and Bockting [7]. No ecotoxicological data were available for 2-chloro-1,3-butadiene and therefore Van de Plassche and Bockting [7] neither derived MPC_{eco} -values nor did they carry out a harmonisation procedure for this chemical. These three substances will not be further discussed in the present report.

Data sets on the other volatiles have been summarised in appendix I, tables 5 (volatile physico-chemical parameters) and 6 (limit values). From these tables it can be seen that the status of the available data (especially the sets of MPCs) is different for the various substances.

- Harmonised substances

For 18 substances harmonised sets of MPCs have been determined [7]. For these substances sufficient data were available to make full eco- and human toxicological evaluations⁷.

Not-harmonised substances

For the remaining 27 substances only sets of preliminary MPCs were derived. For none of these substances MPCs were adjusted downwards, except for 1,3-dichloropropane for which the same MPC_{eco} as for 1,2-dichloropropane were set⁸. For

⁷ In practice, for the report of Van de Plassche and Bockting [7] the harmonisations for these chemicals were carried out on the basis of either (preliminary) NC_{air} or "target values" (i.e. toxicologically based "Negligible Concentrations" in air) which were accepted by Dutch authorities [5,6,29]. Because of linearity of the "SimpleBox" model it makes no difference whether the harmonisation procedure is carried out using NC_{air} s or MPC_{air} s, provided that for the other environmental compartments the corresponding values are used (i.e. taking into account the factor of 100 difference). Calculations in the present report will be carried out with the MPCs.

Ethylene is a special case. For this substance neither an $MCP_{air, human}$ or an NC have been derived, but for this substance a "limit value in air" of $30 \mu\text{g}/\text{m}^3$ (24 hrs average concentration; more or less comparable to $MPC_{air, human}$; see ref 7) has been set. This limit value will be used in the present report.

⁸ For several of these 27 substances $C_{ss,air}$ greatly exceeded the $MPC_{air, human}$. Not adjusting was justified because for these substances insufficient human toxicity data were available which led to application of high uncertainty factors in the derivation of $MPC_{air, human}$. For instance, for 1,1,1-trichloroethane the ratio of $C_{ss,air}$ over $MPC_{air, human}$ was 2100. However, no adjustment was carried out, because the uncertainty factor used in the derivation of this $MPC_{air, human}$ was 10000 [5,7].

five of these substances (2,3-dichloropropene, pentachloroethane, 1,3-dichlorobenzene, 4-chlorotoluene and 3-chlorotoluene), an $MPC_{air, human}$ is not available.

Thus for all but five of these substances, whether their sets of MPCs are harmonised or not-harmonised, sufficient data are available to calculate an EATDE. The calculations are carried out under the assumption that in all environmental compartments the MPCs are reached, simultaneously.

4.1.2 PAHs

An overview of the available data is presented in appendix I, tables 7 (physico-chemical parameters) and 8 (limit values).

For eight of the ten selected PAHs ecotoxicologically based MPCs for water have been derived from experimental data. For the remaining two similar MPCs have been calculated using QSARs, because of a lack of experimental data. Applying equilibrium partitioning for each of these 10 PAHs an MPC_{soil} and MPC_{sed} were calculated, based on the individual MPC_{water} . For three of the PAHs, however, an MPC_{soil} could be derived from experimental data. For these three PAHs the final MPC_{soil} was set at the lowest value of either the experimentally based or the MPC_{water} -derived MPC_{soil} .

Next, using the "SimpleBox" model [8] for each individual PAH the Critical Concentration in air (= CCa) was calculated, which is the steady-state concentration in air in equilibrium with MPC_{soil} ⁹. In these model calculations, primary emission route to air was assumed, which in the case of PAHs is a realistic assumption¹⁰ [27]. Thus for each PAH a set of four values (CCa, MPCs for water, soil and sediment) are obtained which can be considered as a harmonised set of MPCs based on ecotoxicological criteria. A more detailed explanation of the procedure with respect to PAHs has been given in [21] and [28].

For individual PAHs no $MPC_{air, human}$ are available. The Integrated Criteria Document on PAHs [27] only stated that for emissions resulting from combustion of coal "*based on various epidemiological studies, benzo(a)pyrene concentrations ranging from 0.002 to 0.02 ng/m³ correspond to an additional life-time risk of 1 per 10⁶ life-time exposed people. When weighing the different estimates and calculation methods in those studies, a value of 0.01 ng benzo(a)pyrene/m³ (as indicator of the overall group of carcinogens in those mixtures) is probably the most appropriate value to be used in practice*". The $MPC_{air, human}$, associated with a cancer risk of 1 per 10⁴ life-time exposed people is 1 ng benzo(a)pyrene/m³, which concentration is adopted in The Netherlands as the "limit value" for benzo(a)pyrene in air as indicator value for "total PAHs" [29]. The assumption that the $MPC_{air, human}$ of 1 ng/m³ for benzo(a)pyrene also applies to the other PAHs (i.e. their individual $MPC_{air, human}$ are also 1 ng/m³) would

⁹ CCa is a "critical" concentration because if this concentration is exceeded the MPC_{soil} will be exceeded to as a result of deposition.

The CCa for PAHs is calculated only for the soil compartment, because a) for PAH MPC_{soil} are derived from MPC_{water} using equilibrium partitioning and b) in water PAH only occur absorbed to the sediment fraction thus with negligible concentrations of free PAHs (personal communication, Kalf, 1998).

The reason why the CCa for metals is calculated only for the soil compartment cannot be recovered.

¹⁰ This assumption differs from the one for volatile substances, because for the latter group Steady-state concentrations were calculated assuming emission to water [7].

probably result in an over-estimation of the inhalatory cancer-risk for the other PAHs, as their carcinogenic potencies are probably not higher than that of benzo(a)pyrene [27].

4.1.3 metals

An overview of the data is presented in appendix I, tables 9, (physico-chemical parameters), 10 (ecological limit values) and 11 (human limit values and bioaccumulation factors for human dietary constituents).

For some 20 metals MPC_{eco} are available [22]. Given the data as mentioned in the respective tables on metals in appendix I, it can be seen that estimation of human exposure to metals with the EUSES program based on their respective MPC_{eco} s will be highly uncertain. For this uncertainty several reasons exist:

- metals do not occur in the environment in one single chemical form (speciation). The actual speciation in which the metal occurs depends on e.g. oxidation status and pH of the medium (soil or water). Changes in chemical speciation will result in changes in chemical characteristics [21, 30]. In the EUSES or the "SimpleBox" model system only for one chemical speciation at a time physico-chemical data can be entered. For CrIII, CrVI, Hg and methyl-Hg separate MPC_{eco} s were calculated. For the other metals speciation was not taken into account¹¹ [22].
- In order to estimate human exposure, EUSES calculates accumulation and transfer of substances through the human food chain on the basis of K_{ow} . For metals the basic physico-chemical data required for EUSES calculations are lacking: for most metal (speciations) H_c , SOL and K_{ow} are irrelevant or non-existing. Although the physico-chemical characteristics as presented in appendix I, table 9 can be entered into the EUSES programme the programme results will be unreliable (e.g. ref. 20). Alternatively, actual bioaccumulation factors (BCFs), which have been determined in field of laboratory experiments can be used [20].
- For animals used for human consumption only transfer factors, comparable to BCFs were located for lead. Although for several other metals incidental (qualitative) remarks on transfer to e.g. milk or meat were found [31], quantitative data are not present.
For plants and fish bioaccumulation data are somewhat more abundant, although either incomplete (e.g. fish; Drs C. van der Guchte, RIZA, Lelystad and Dr. F Swartjes, RIVM-LBG, Bilthoven, personal communications, 1997) or representatives of a broad range of estimates (e.g. plants; refs. 12, 32). In both cases considerable uncertainty with respect to the accuracy of these bioaccumulation factors must be taken into account.
- EUSES computes an EATDE by summation of intake via oral and inhalatory routes. For several metals comparatively large differences in bioavailability for these routes have been mentioned indicating that uptake after inhalation is much higher than uptake after oral exposure [31]. Whether sufficiently accurate estimates of bioavailability are available is at the moment unclear.

¹¹ Toxicity tests are usually carried out with a limited choice of very soluble salts (e.g. $CdCl_2$ and $CdNO_3$, or $CuSO_4$ and $CuCl_2$).

The CCa-s which are adherent to the ecotoxicologically based MPC_{soil} s for the various metals were derived following the assumption that the main route of emission is to air (primary compartment)^{9, 10} [22].

For all metals human limit values (in the form of MPRs) have been derived, but only for a few of them MPC_{air} have been defined. Whether inhalatory exposure of the general population to metals is of toxicological relevance can only be assessed for these few metals.

4.2 Conclusions: data availability and feasibility of human exposure assessment.

1. For all of the substances of interest, ecotoxicologically based MPCs have been derived. Availability of physico-chemical parameters is limited for metals and availability of human limit values is limited for metals, PAHs and a number of volatile substances.
2. Only for 18 volatile substances complete sets of MPCs air, soil, water and sediment (including $MPC_{air, human}$) were derived. For these 18 substances multi-route exposure calculations for humans are possible and the estimated EATDEs may be indicative for a health risk for the general population.
3. For 22 volatile substances only preliminary $MPC_{air, human}$ were available. For none of these, harmonisation of MPC has taken place, despite the fact that in some cases the calculated C_{ss} in air was considerably higher than the preliminary $MPC_{air, human}$. The present $MPC_{air, human}$ were preliminary because of a lack of data leading to high uncertainty factors [5,6,7]. Whether for these 22 substances fully harmonised MPCs can be derived in future depends on if $MPC_{air, human}$ with a more conclusive will become available. For these substances multi-route exposure calculations for humans are possible, but with respect to toxicological interpretability (i.e. indicative value for health risk) the results are of less value than for the other 18 volatiles.
4. RIVM did not derive $MPC_{air, human}$ or preliminary $MPC_{air, human}$ for five chemicals namely 2,3-dichloropropene, pentachloroethane, 1,3-dichlorobenzene, 4-chlorotoluene and 3-chlorotoluene. Therefore, neither a full multi-route exposure estimation can be calculated, nor is it possible to carry out a human health risk assessment under the current concept.
5. For PAHs sufficient physico-chemical data are available. Human limit values are available as MPR. For inhalatory exposure, only a group $MPC_{air, human}$ is available, for which benzo(a)pyrene is used as a guidance substance.
6. For metals a very first survey can be made, but the results will be extremely premature because of lack of data and/or models which allow for estimation of total human daily intake. The major data gaps are in the field of transfer of metals through the human food chain. As a start, for metals transfer may be modelled using the BCFs for lead but it is unlikely that this may provide results with sufficient scientific quality.

4.3 Consequences of data limitations

The conclusions presented in section 4.2 and the information as presented in paragraphs 4.1.1 through 4.1.3 were discussed in a project steering group meeting (Ministry of VROM, directorate SVS, June, 18, 1997). At this meeting it was decided to perform multi-route exposure estimation and assessment of human health risk only for the volatile substances for which complete data sets (either preliminary or harmonised) are available, and for benzo(a)pyrene.

5. Risk and exposure patterns: results and discussion

As indicated in section 4.3, because of inadequate data or limited data availability for metals and PAHs, in this chapter exposure estimates are calculated, for the volatile organic substances and benzo(a)pyrene, only. The results of these calculations have been presented in tables 1 to 3. Furthermore, to gain some insight into the relevance of the various routes of exposure, frequency distributions have been made of the routes via air, water and diet (all constituents summed). These frequency distributions have been presented in figures 2a to 2c.

Subsequently, a comparison is made between the human multi-route exposure patterns obtained in the present report and the human multi-route exposure patterns obtained in the IV-project.

5.1 Estimation of human average daily exposure and risk.

5.1.1 estimated average total daily exposure

The estimated average total daily exposure (EATDE) for the substances studied has been calculated as the sum of the exposures via the various routes (table 1). This EATDE can be considered as an estimate of total internal exposure (uptake) because bioavailability was taken into account (albeit as defaults i.e. 100% available for the oral routes and 75% available via inhalation).

Because of the assumption of 100% oral bioavailability, the EATDE can also be considered as an equivalent of daily oral exposure, and as such it can be compared to MPR values, resulting in a ratio EATDE/MPR, which indicates if the EATDE exceeds the MPR and thus the possibility of a risk. However, such a comparison is only valid if the MPR has been defined for systemic effects and local effects such as corrosivity / irritation or exposure site-specific carcinogenicity are irrelevant. Thus, the type of effect after either inhalatory or oral exposure has been taken into account. Except for benzo(a)pyrene, for all substances the MPR was based on systemic effects, which allows direct comparison of MPR and EATDE. The MPR for benzo(a)pyrene has been based on local (i.e. fore-stomach) tumours. Therefore, for this substance the ratio EATDE/MPR was calculated for the oral part of the EATDE, only. However, in practice, inclusion of the inhalatory contribution to the EATDE for benzo(a)pyrene would not have resulted in a ratio EATDE/MPR greatly differing from the present one because inhalatory exposure contributes only for less than 1 % to the EATDE for benzo(a)pyrene.

5.1.2 Human health risk assessment

The MPRs used for calculation of the ratio EATDE/MPR (table 2) are the same as those used for derivation of soil clean-up Intervention Values. For a number of chemicals (1,3-dichloropropene, 3-chloropropene, ethylene, ethylene oxide, 1,1,2,2-tetrachloroethane and hexachloroethane) no MPR has been derived by RIVM. In order to give a rough impression of a possible risk a quick scan was made to find MPRs (or similar values) derived by other organisations (e.g. EPA-IRIS, ATSDR, WHO).

Table 1. Multi-route estimates of average daily exposure and estimates of average total daily exposure (EATDE) to environmental contaminants under the assumption that concentrations in the environment are equal to the MPCs derived for air, water, sediment or soil.

| substance | Estimated average daily exposure via ($\mu\text{g}/\text{kg bw}/\text{d}$) | | | | | | | | EATDE ($\mu\text{g}/\text{kg bw}/\text{d}$) |
|----------------------------------|---|------|------------|------------|------|------|---------|------|--|
| | drinking water | fish | leaf crops | root crops | meat | milk | air | soil | |
| harmonised volatiles | | | | | | | | | |
| 1,1,1-trichloroethane | 60.00 | 8.61 | 0.26 | 15.80 | 0.00 | 0.03 | 1030.00 | 0.00 | 1114.71 |
| 1,1-dichloroethylene | 97.10 | 4.06 | 0.00 | 10.60 | 0.00 | 0.00 | 42.90 | 0.01 | 154.68 |
| 1,2-dichloroethane | 20.00 | 0.40 | 0.01 | 1.60 | 0.00 | 0.00 | 21.40 | 0.00 | 43.41 |
| 1,2-dichloropropane | 2.17 | 0.12 | 0.00 | 0.27 | 0.00 | 0.00 | 2.57 | 0.00 | 5.13 |
| 1,3-dichloropropene | 0.23 | 0.00 | 0.01 | 0.02 | 0.00 | 0.00 | 8.57 | 0.00 | 8.84 |
| 3-chloropropene | 0.10 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.59 | 0.00 | 1.70 |
| acrylonitrile | 0.22 | 0.00 | 0.03 | 0.01 | 0.00 | 0.00 | 2.14 | 0.00 | 2.40 |
| benzene | 6.86 | 0.55 | 0.00 | 1.13 | 0.00 | 0.00 | 6.43 | 0.00 | 14.97 |
| dichloromethane | 571.00 | 7.24 | 0.27 | 40.70 | 0.00 | 0.06 | 364.00 | 0.00 | 983.26 |
| ethylene | 243.00 | 2.43 | 0.00 | 16.50 | 0.00 | 0.02 | 6.43 | 0.00 | 268.38 |
| ethylene oxide | 2.40 | 0.02 | 0.00 | 0.14 | 0.00 | 0.00 | 0.64 | 0.00 | 3.20 |
| styrene | 16.30 | 5.75 | 0.23 | 10.10 | 0.00 | 0.00 | 171.00 | 0.02 | 203.41 |
| tetrachloroethylene ¹ | 9.43 | 8.03 | 0.87 | 14.70 | 0.04 | 0.04 | 536.00 | 0.00 | 569.10 |

Estimated average daily exposure via
(µg/kg bw/d)

EATDE
(µg/kg bw/d)

| substance | Estimated average daily exposure via | | | | | | | EATDE (µg/kg bw/d) | |
|----------------------------------|--------------------------------------|-------|------------|------------|------|------|---------|-----------------------|---------|
| | drinking water | fish | leaf crops | root crops | meat | milk | air | | soil |
| tetrachloroethylene ² | 9.43 | 8.03 | 0.09 | 14.70 | 0.00 | 0.00 | 53.60 | 0.00 | 85.86 |
| tetrachloromethane | 31.40 | 8.77 | 0.00 | 15.40 | 0.00 | 0.00 | 12.90 | 0.03 | 68.51 |
| toluene | 20.90 | 5.38 | 0.07 | 9.46 | 0.00 | 0.00 | 64.30 | 0.00 | 100.11 |
| trichloroethylene | 68.60 | 8.58 | 0.65 | 16.00 | 0.00 | 0.03 | 1070.00 | 0.01 | 1163.87 |
| trichloromethane | 16.90 | 0.87 | 0.01 | 0.00 | 0.00 | 0.00 | 21.40 | 0.00 | 39.19 |
| vinylchloride | 23.40 | 0.05 | 0.00 | 1.93 | 0.00 | 0.00 | 21.40 | 0.00 | 46.78 |
| <i>PAHs</i> | | | | | | | | | |
| benzo(a)pyrene | 0.00 | 0.19 | 0.01 | 0.59 | 0.01 | 0.01 | 0.00 | 0.00 | 0.81 |
| preliminary | | | | | | | | | |
| 1,1,2,2-tetrachloroethane | 94.30 | 11.10 | 0.00 | 21.00 | 0.00 | 0.00 | 0.04 | 0.01 | 126.47 |
| 1,1,2-trichloroethane | 226.00 | 10.00 | 0.02 | 25.50 | 0.00 | 0.02 | 3.86 | 0.03 | 265.43 |
| 1,1-dichloroethane | 20.00 | 0.73 | 0.02 | 2.04 | 0.00 | 0.00 | 79.30 | 0.00 | 102.09 |
| 1,2,3,4-tetrachlorobenzene | 0.69 | 6.61 | 0.23 | 15.60 | 0.00 | 0.00 | 0.34 | 0.00 | 23.49 |
| 1,2,3,5-tetrachlorobenzene | 0.69 | 6.88 | 0.15 | 660.00 | 0.00 | 0.00 | 0.34 | 0.00 | 668.07 |
| 1,2,3-trichlorobenzene | 1.91 | 6.94 | 0.05 | 14.60 | 0.00 | 0.00 | 0.86 | 0.00 | 24.36 |
| 1,2,4,5-tetrachlorobenzene | 0.69 | 6.12 | 0.16 | 14.30 | 0.00 | 0.00 | 0.34 | 0.00 | 21.62 |
| 1,2,4-trichlorobenzene | 1.91 | 5.82 | 0.04 | 12.00 | 0.00 | 0.00 | 0.86 | 0.00 | 20.63 |
| 1,2-dichlorobenzene | 7.14 | 6.45 | 0.11 | 11.90 | 0.00 | 0.03 | 12.90 | 0.00 | 38.53 |
| 1,2-dichloroethylene | 174.00 | 7.29 | 0.00 | 19.10 | 0.00 | 0.02 | 7.71 | 0.02 | 208.14 |

| substance | Estimated average daily exposure via ($\mu\text{g}/\text{kg bw}/\text{d}$) | | | | | | | | EATDE ($\mu\text{g}/\text{kg bw}/\text{d}$) |
|------------------------|---|------|------------|------------|-------|-------|--------|------|--|
| | drinking water | fish | leaf crops | root crops | meat | milk | air | soil | |
| 1,2-xylene | 10.90 | 5.35 | 0.20 | 9.48 | 0.00 | 0.00 | 72.90 | 0.01 | 98.84 |
| 1,3-dichloropropane | 2.17 | 0.12 | 0.00 | 0.28 | 0.00 | 0.05 | 2.57 | 0.00 | 5.19 |
| 1,3,5-trichlorobenzene | 0.69 | 6.88 | 0.15 | 660.00 | 0.00 | 0.00 | 0.34 | 0.00 | 668.07 |
| 1,3-xylene | 10.90 | 6.25 | 0.50 | 11.20 | 0.01 | 0.01 | 214.00 | 0.01 | 242.88 |
| 1,4-dichlorobenzene | 7.14 | 6.58 | 1.03 | 12.00 | 0.01 | 0.01 | 144.00 | 0.00 | 170.78 |
| 1,4-xylene | 10.90 | 5.73 | 0.41 | 10.10 | 0.00 | 0.00 | 214.00 | 0.01 | 241.17 |
| 2-chlorotoluene | 8.86 | 6.45 | 0.40 | 11.70 | 0.01 | 0.01 | 167.00 | 0.02 | 194.46 |
| ethylbenzene | 10.60 | 5.52 | 0.02 | 9.81 | 0.00 | 0.00 | 8.36 | 0.00 | 34.31 |
| hexachlorobenzene | 0.07 | 5.58 | 5.12 | 16.90 | 51.80 | 51.60 | 0.49 | 0.00 | 131.56 |
| hexachloroethane | 2.37 | 8.60 | 0.07 | 18.10 | 0.00 | 0.00 | 5.79 | 0.01 | 34.96 |
| monochlorobenzene | 19.70 | 6.31 | 0.02 | 11.10 | 0.00 | 0.00 | 9.00 | 0.01 | 46.14 |
| pentachlorobenzene | 0.21 | 5.95 | 2.79 | 15.80 | 0.26 | 0.26 | 1.71 | 0.00 | 26.98 |

1,2 For tetrachloroethylene two sets of estimates of average daily exposure have been given. The one indexed with 1 results from the previous $\text{MPC}_{\text{air, human}}$ of 2500 $\mu\text{g}/\text{m}^3$. The one indexed with 2 results from the recently updated $\text{MPC}_{\text{air, human}}$ of 250 $\mu\text{g}/\text{m}^3$.

No MPR could be found for 3-chloropropene, ethylene and ethylene oxide. For these substances a provisional estimate of an MPR was derived from the $MPC_{air, human}$ following route-to-route extrapolation assuming 75 % bioavailability after inhalation, 100% bioavailability after oral exposure, a respiratory volume of $20 \text{ m}^3/\text{d}$ and an average adult body weight of 70 kg^{12} . The (estimated) MPR s for these 7 chemicals have been incorporated in the present report, however, without any further validation and should be treated with great caution!

Table 2 shows that for only 5 substances (benzo(a)pyrene, 1,2-dichloropropane, toluene, ethylbenzene and monochlorobenzene) the MPR will not be exceeded (i.e. their ratios EATDE/MPR are less than unity) if their concentrations in the environment are maintained at the MPC-levels as presented in appendix I. For 11 chemicals the ratio EATDE/MPR was between 1 and 10 and for all others (25 substances) these ratios were above 10; for four of these (1,2,3,5-tetrachlorobenzene, 1,3,5-tetrachlorobenzene, 1,4-dichlorobenzene and hexachlorobenzene) even above 100.

Interestingly, the four chlorobenzenes for which a ratio EADTE/MPR > 100 was found, all have the same MPR of $0.5 \text{ } \mu\text{g}/\text{kg b.w./d}$, which because of lack of data was set equal to the one derived for hexachlorobenzene. This was done because hexachlorobenzene is relatively well studied and the most toxic congener [33]. This may lead of course to an over-estimation of the toxicological risk of these substances for humans.

For tetrachloroethylene two exposure scenarios have been studied. Because in the course of this research the $MPC_{air, human}$ was lowered by a factor of ten to $250 \text{ } \mu\text{g}/\text{m}^3$ (see ref. 34; value adopted by RIVM), the ministry requested to perform an additional harmonisation and exposure calculation to evaluate the compatibility of this new $MPC_{air, human}$ with the existing MPCs for the other compartments. Following the same procedure as described in Van de Plassche and Bockting [7], the updated MPC was also compatible with the previously reported MPCs for water, soil and sediment. In other words: these MPCs combined with the updated $MPC_{air, human}$ can still be considered a harmonised set of MPCs. However, although lowering of the $MPC_{air, human}$ for tetrachloroethylene from 2500 to $250 \text{ } \mu\text{g}/\text{m}^3$ reduces the EATDE from 569 to $86 \text{ } \mu\text{g}/\text{kg b.w./d}$, the MPR for this substance will still be exceeded by a factor of ca. 5 (see table 1 and 2).

Recently RIVM has derived an updated $MPC_{air, human}$ for 1,1-dichloroethylene of $14 \text{ } \mu\text{g}/\text{m}^3$ [35]. However, in concordance with the previous reports in this series (see ref. 7), all calculations for the present report have been carried out using the earlier derived $MPC_{air, human}$ of $200 \text{ } \mu\text{g}/\text{m}^3$ [6]. Based on this new $MPC_{air, human}$ for 1,1-dichloroethylene an EATDE of $115 \text{ } \mu\text{g}/\text{kg b.w./d}$ would have been calculated, resulting in a ratio EATDE/MPR of approximately 40.

¹² This is only allowed if the $MPC_{air, human}$ is based on systemic effects, which is the case for 3-chloropropene and ethylene oxide [6,25]. An $MPC_{air, human}$ for ethylene has not been derived (see under footnote 2), but for this chemical only systemic effects have been described [26].

Table 2. Comparison of EATDE and MPR for exposure of humans to contaminants at MPCs derived for air, water, sediment and soil.

| substance | EATDE [@] µg/kg b.w./d | MPR [@] µg/kg b.w./d | | ratio [@] EATDE/MPR |
|-----------------------------------|------------------------------------|----------------------------------|-----------|---------------------------------|
| | | value | source | |
| harmonised | | | | |
| <i>volatiles</i> | | | | |
| 1,1,1-trichloroethane | 1114.71 | 80 | [36], rtr | 13.9 |
| 1,1-dichloroethylene | 154.67 | 3 | [35] | 51.6 |
| 1,2-dichloroethane | 43.41 | 14 | [33], rtr | 3.1 |
| 1,2-dichloropropane | 5.13 | 70 ^a | [35] | 0.07 |
| 1,3-dichloropropene | 969.27 | 67 ^a | [37] | 14.5 |
| 3-chloropropene | 1.70 | 16.7 ^b | rtr | 0.1 |
| acrylonitrile | 2.40 | 0.1 | [35] | 24 |
| benzene | 14.97 | 4.3 | [38], rtr | 3.5 |
| dichloromethane | 983.26 | 60 | [33] | 16.4 |
| ethylene | 268.38 | 6400 ^b | rtr | 0.04 |
| ethylene oxide | 3.20 | 0.64 ^b | rtr | 5 |
| styrene | 203.39 | 77 | [33] | 2.6 |
| tetrachloroethylene ^{1c} | 569.10 | 16 | [33] | 35.6 |
| tetrachloroethylene ^{2c} | 85.86 | 16 | [33] | 5.4 |
| tetrachloromethane | 68.48 | 4 | [33] | 17.1 |
| toluene | 100.11 | 430 | [33], rtr | 0.23 |
| trichloroethylene | 1163.87 | 540 | [33], rtr | 2.2 |
| trichloromethane | 39.19 | 30 | [33] | 1.3 |
| vinylchloride | 46.78 | 3.51 | [33] | 13.3 |
| <i>PAHs</i> | | | | |
| benzo(a)pyrene | 0.81 | 2 - 4 | [33] | 0.4 - 0.2 |
| preliminary | | | | |
| 1,1,2,2-tetrachloroethane | 126.46 | 3 ^a | [39] | 42.2 |
| 1,1,2-trichloroethane | 265.40 | 4 ^f | [35] | 66.4 |
| 1,1-dichloroethane | 102.09 | 80 | [36], rtr | 1.3 |
| 1,2,3,4-tetrachlorobenzene | 23.49 | 0.5 | [33] | 47.0 |
| 1,2,3,5-tetrachlorobenzene | 668.07 | 0.5 | [33] | 1336 |
| 1,2,3-trichlorobenzene | 24.36 | 0.5 | [33] | 48.7 |
| 1,2,4,5-tetrachlorobenzene | 21.62 | 0.5 | [33] | 43.2 |
| 1,2,4-trichlorobenzene | 20.63 | 0.5 | [33] | 41.3 |
| 1,2-dichlorobenzene | 38.53 | 0.5 | [33] | 77.1 |
| 1,2-dichloroethylene | 208.12 | 6 ^e | [36] | 34.7 |

| substance | EATDE [@] µg/kg b.w./d | MPR [@] µg/kg b.w./d | | ratio [@] EATDE/MPR |
|------------------------|------------------------------------|----------------------------------|--------|---------------------------------|
| | | value | source | |
| 1,2-xylene | 98.83 | 10 | [33] | 9.9 |
| 1,3-dichloropropane | 5.19 | 50 | [35] | 0.1 |
| 1,3,5-trichlorobenzene | 668.07 | 0.5 | [33] | 1340 |
| 1,3-xylene | 242.87 | 10 | [33] | 24.3 |
| 1,4-dichlorobenzene | 170.78 | 0.5 | [33] | 340 |
| 1,4-xylene | 241.16 | 10 | [33] | 24.1 |
| 2-chlorotoluene | 194.44 | 20 | [40] | 9.7 |
| ethylbenzene | 34.31 | 136 | [33] | 0.3 |
| hexachlorobenzene | 131.56 | 0.5 | [33] | 260 |
| hexachloroethane | 34.95 | 1 ^a | [41] | 35.0 |
| monochlorobenzene | 46.13 | 0.5 | [33] | 92.3 |
| pentachlorobenzene | 26.98 | 0.5 | [33] | 54.0 |

@ Abbreviations: EATDE: estimated average total daily intake; MPR: maximum tolerated risk level;

- a For these substances no MPRs were derived by RIVM. However, MPRs or comparable values were derived by other organisations. In order to give a rough impression of a possible risk, these values were used here for calculations of the EATDE/MPR ratio. These MPR -values must not be used in policy making before they have been further validated.
- b For 3-chloropropene, ethylene and ethylene oxide an MPR could not be found. The value presented here has been calculated from the MPC_{air, human} assuming a respiration rate of 20 m³/person/day, an inhalatory bioavailability of 75% and a body weight of 70 kg. In order to give a rough impression of a possible risk, this value was used here for the calculation of the EATDE/MPR ratio. The MPR -value must not be used in policy making before it has been further validated.
- c The MPC_{air} for this substance has been reduced from 2500 µg/m³ to 250 µg/m³, recently. Harmonisation and risk assessments have been carried out for both the old (index 1) as well as the new (index 2) MPC_{air}.
- d For BaP the ratio EATDE/MPR has been calculated for the oral contribution to EATDE, because the effect is based on local tumours (i.e. tumours of the fore-stomach in rats). The oral routes contributes to the EATDE for > 99 % (see table 3).
- e The given toxicological health advisory for 1,2 dichloroethylene pertains to the cis-isomer. The MPR for the trans-isomer is about a factor of three higher.
- f The MPR for 1,1,2-trichloroethane is provisional.

5.2 Multi-route exposure patterns

Table 3 provides an overview of the contribution of the various routes of exposure to the EATDE, showing their relevance in the multi-route exposure pattern. Frequency distributions and relative cumulative distributions for exposure via air, water and food (all components summed) are given in figures 2a to 2c.

Although it was expected that for less volatile substances (e.g. benzo(a)pyrene, hexachlorobenzene) exposure via soil uptake would contribute to a large extent to EATDE, even for these substances, contribution via this route is negligible (table 3). Uptake of soil contaminants may, however, be relevant by carry-over via the human food chain (uptake by plants). From table 1 and 3 it may be concluded that for some substances this carry-over may be quite extensive (especially for root crops e.g. 1,3,5-tri- and 1,2,3,5-tetrachlorobenzene) if the soil pore water concentration is equal to the MPC_{water} . From table 4 it can be concluded that carry-over via plants which is calculated by the computer model, is highly dependent on the concentration of substances in the soil pore water and less or independent on the concentration in soil. The situation in table 4 with zero groundwater concentration (the numbers printed in bold typeface) is highly artificial, because in practice the concentration in soil water will be roughly in equilibrium with the concentration in soil.

In contrast to the previous version of EUSES 1.0 (i.e. USES 1.0) the transfer of air contaminants to overground plant parts is limited to gaseous uptake from air. In USES 1.0 deposition of aerosols on plants contributes to human exposure, too. According to McLachlan [42] for chlorinated dibenzodioxins, dibenzofurans and biphenyls aerosol deposition may be more relevant for accumulation of air contaminants in plants than gaseous air/plant partitioning. So, concentrations of overground plant parts may be underestimated in the present model, which results in an under-estimation of the relevance of human exposure via the plant (shoots).

Another rather unexpected result was the fact that given the sets of MPCs, for many of these substances inhalation is not the major route of exposure. If ever concentrations in all environmental compartments would be equal to these MPCs simultaneously, the 50th-percentile lays at 40 % meaning that for some 20 out of 40 substances inhalation contributes to less than 40 % to EATDE. Substances falling within this 50th-percentile are by no means the least volatile¹³ ones per se, e.g. 1,1-dichloroethylene, 1,2-dichloroethylene, ethylene or ethylbenzene.

For *ca.* 40 % of the substances exposure via water contributes to 25% or more to the EATDE while for *ca.* 35 % of the substances dietary contribution is 25% or more. In the latter percentage ($\geq 25\%$ via diet), exposure via plant and animal products have been summed. However, exposure via milk or meat is only important for one substance: hexachlorobenzene. In analogy with lipophilic halogenated aromatics such

¹³ Here "volatile" refers to vapour pressure. For environmental distribution of substances, air/water- and air/soil-partition coefficients are also important.

Table 3. Relative contribution of separate routes of exposure to estimated average total daily exposure

| substance | percentage of Estimated Average Total Daily Exposure (EATDE) | | | | | | | |
|----------------------------------|--|------|------------|------------|------|------|-------|------|
| | drinking water | fish | leaf crops | root crops | meat | milk | air | soil |
| harmonised volatiles | | | | | | | | |
| 1,1,1-trichloroethane | 5.38 | 0.77 | 0.02 | 1.42 | 0.00 | 0.00 | 92.40 | 0.00 |
| 1,1-dichloroethylene | 62.78 | 2.62 | 0.00 | 6.85 | 0.00 | 0.00 | 27.74 | 0.01 |
| 1,2-dichloroethane | 46.07 | 0.92 | 0.03 | 3.69 | 0.00 | 0.00 | 49.29 | 0.00 |
| 1,2-dichloropropane | 42.27 | 2.28 | 0.05 | 5.34 | 0.00 | 0.00 | 50.06 | 0.06 |
| 1,3-dichloropropene | 2.59 | 0.09 | 0.12 | 0.26 | 0.00 | 0.00 | 96.94 | 0.00 |
| 3-chloropropene | 5.72 | 0.11 | 0.02 | 0.45 | 0.00 | 0.00 | 93.69 | 0.00 |
| acrylonitrile | 9.04 | 0.07 | 1.18 | 0.53 | 0.00 | 0.00 | 89.17 | 0.00 |
| benzene | 45.82 | 3.65 | 0.02 | 7.55 | 0.00 | 0.00 | 42.95 | 0.00 |
| dichloromethane | 58.07 | 0.74 | 0.03 | 4.14 | 0.00 | 0.00 | 37.02 | 0.00 |
| ethylene | 90.54 | 0.91 | 0.00 | 6.15 | 0.00 | 0.01 | 2.40 | 0.00 |
| ethylene oxide | 74.98 | 0.58 | 0.00 | 4.34 | 0.00 | 0.01 | 20.09 | 0.00 |
| styrene | 8.01 | 2.83 | 0.11 | 4.97 | 0.00 | 0.00 | 84.08 | 0.01 |
| tetrachloroethylene ¹ | 1.66 | 1.41 | 0.15 | 2.58 | 0.01 | 0.01 | 94.18 | 0.00 |
| tetrachloroethylene ² | 10.98 | 9.35 | 0.1 | 17.12 | 0.01 | 0.01 | 62.43 | 0.00 |

percentage of Estimated Average Total Daily Exposure (EATDE)

| substance | drinking | fish | leaf crops | root crops | meat | milk | air | soil |
|----------------------------|----------|-------|------------|------------|------|------|-------|------|
| | water | | | | | | | |
| tetrachloromethane | 45.85 | 12.81 | 0.01 | 22.49 | 0.00 | 0.01 | 18.84 | 0.04 |
| toluene | 20.88 | 5.37 | 0.07 | 9.45 | 0.00 | 0.00 | 64.23 | 0.00 |
| trichloroethylene | 5.89 | 0.74 | 0.06 | 1.37 | 0.00 | 0.00 | 91.93 | 0.00 |
| trichloromethane | 43.12 | 2.23 | 0.04 | 0.01 | 0.00 | 0.01 | 54.60 | 0.00 |
| vinylchloride | 50.02 | 0.11 | 0.00 | 4.13 | 0.00 | 0.01 | 45.74 | 0.00 |
| <i>PAHs</i> | | | | | | | | |
| benzo(a)pyrene | 0.18 | 22.83 | 1.45 | 72.90 | 1.33 | 1.33 | 0.00 | 0.08 |
| preliminary | | | | | | | | |
| 1,1,2,2-tetrachloroethane | 74.57 | 8.78 | 0.01 | 16.61 | 0.00 | 0.01 | 0.03 | 0.01 |
| 1,1,2-trichloroethane | 85.16 | 3.77 | 0.01 | 9.61 | 0.00 | 0.01 | 1.45 | 0.01 |
| 1,1-dichloroethane | 19.59 | 0.71 | 0.02 | 2.00 | 0.00 | 0.00 | 77.67 | 0.00 |
| 1,2,3,4-tetrachlorobenzene | 2.92 | 28.14 | 0.98 | 66.42 | 0.04 | 0.04 | 1.46 | 0.00 |
| 1,2,3,5-tetrachlorobenzene | 0.10 | 1.03 | 0.02 | 98.79 | 0.00 | 0.00 | 0.05 | 0.00 |
| 1,2,3-trichlorobenzene | 7.84 | 28.49 | 0.18 | 59.94 | 0.01 | 0.01 | 3.52 | 0.00 |
| 1,2,4,5-tetrachlorobenzene | 3.17 | 28.31 | 0.74 | 66.14 | 0.03 | 0.03 | 1.59 | 0.00 |
| 1,2,4-trichlorobenzene | 9.26 | 28.21 | 0.18 | 58.17 | 0.01 | 0.01 | 4.15 | 0.00 |
| 1,2-dichlorobenzene | 18.53 | 16.74 | 0.29 | 30.88 | 0.00 | 0.07 | 33.48 | 0.00 |
| 1,2-dichloroethylene | 83.60 | 3.50 | 0.00 | 9.18 | 0.00 | 0.00 | 3.70 | 0.02 |

percentage of Estimated Average Total Daily Exposure (EATDE)

| substance | drinking | fish | leaf crops | root crops | meat | milk | air | soil |
|------------------------|----------|-------|------------|------------|-------|-------|-------|------|
| | water | | | | | | | |
| 1,2-xylene | 11.03 | 5.41 | 0.20 | 9.59 | 0.00 | 0.00 | 73.76 | 0.01 |
| 1,3-dichloropropane | 41.84 | 2.29 | 0.03 | 5.36 | 0.00 | 0.92 | 49.55 | 0.00 |
| 1,3,5-trichlorobenzene | 0.10 | 1.03 | 0.02 | 98.79 | 0.00 | 0.00 | 0.05 | 0.00 |
| 1,3-xylene | 4.49 | 2.57 | 0.20 | 4.61 | 0.00 | 0.00 | 88.11 | 0.00 |
| 1,4-dichlorobenzene | 4.18 | 3.85 | 0.60 | 7.03 | 0.00 | 0.00 | 84.32 | 0.00 |
| 1,4-xylene | 4.52 | 2.38 | 0.17 | 4.19 | 0.00 | 0.00 | 88.74 | 0.00 |
| 2-chlorotoluene | 4.56 | 3.32 | 0.21 | 6.02 | 0.01 | 0.01 | 85.89 | 0.01 |
| ethylbenzene | 30.89 | 16.09 | 0.06 | 28.59 | 0.00 | 0.00 | 24.36 | 0.00 |
| hexachlorobenzene | 0.05 | 4.24 | 3.89 | 12.85 | 39.37 | 39.22 | 0.37 | 0.00 |
| hexachloroethane | 6.78 | 24.61 | 0.19 | 51.79 | 0.03 | 0.03 | 16.57 | 0.03 |
| monochlorobenzene | 42.70 | 13.68 | 0.04 | 24.06 | 0.00 | 0.00 | 19.51 | 0.02 |
| pentachlorobenzene | 0.79 | 22.06 | 10.34 | 58.57 | 0.95 | 0.95 | 6.34 | 0.00 |

1,2 For tetrachloroethylene a set of estimates of average daily exposure have been given for the previous $MPC_{air, human}$ of $2500 \mu\text{g}/\text{m}^3$ and another set has been given for the recently updated $MPC_{air, human}$ of $250 \mu\text{g}/\text{m}^3$ (see table 1). In table 2 relative importance of the identified routes of exposure have been given for 1: pertaining to the previous $MPC_{air, human}$ of $2500 \mu\text{g}/\text{m}^3$ and 2: pertaining to the updated $MPC_{air, human}$ of $250 \mu\text{g}/\text{m}^3$

as chlorinated dibenzodioxines, the importance of the route via animal food products is not unexpected [42, 43].

In those cases where exposure via the diet is important, the highest exposures are observed from consumption of fish or root crops. For pentachlorobenzene, hexachloroethane or tetrachloromethane these routes (together) contribute for *ca.* 80%, 75%, or 45% of EATDE, respectively.

An explanation for the finding that for so many volatile substances other routes than inhalation contribute to the EATDE to such a high degree, may be the fact that apart from environmental behaviour also the toxicity and more in particular the ecotoxicity of the substance is an important factor to determine the height of the MPCs in water or soil. Moreover the assumption underlying the derivation of the harmonised MPCs that for volatile substances emissions are for 100% to water and not to air will also contribute to this finding. Following the latter assumption, the $MPC_{\text{water, eco}}$ will highly affect the calculated exposure patterns, resulting in an exaggerated role for the routes depending on concentration in water (e.g. drinking water, fish, plants).

In order to gain insight in the role of drinking water purification, for eight substances alternative calculations with EUSES were carried out. In these alternative calculations EUSES was forced to use (purified) surface water for drinking water exposure by assuming that no contaminants were present in ground water (i.e. concentration = 0 mg/l).

Five substances were chosen because of paramount importance of the drinking water route (1,1-dichloroethylene to 1,2-dichloroethylene; see table 4).

For these five substances this results in a (sometimes considerable) drop in the EATDE (table 4). However, the relevance of the route via drinking water is not greatly affected and although the percentage of the exposure via air may double in an incidental case it still remains unexpectedly low for these volatile substances. Furthermore it was observed that intake via root crops disappeared.

This effect was further studied for three more substances with very high importance of exposure through root crops (benzo(a)pyrene), or more or less uniform distribution between drinking water, fish, root crops, and air (ethylbenzene, monochlorobenzene). Recalculation with zero groundwater concentrations for these three substances resulted in virtually unchanged relevance of the drinking water route. However exposure through fish gained in importance, while for ethylbenzene and monochlorobenzene exposure through air gained in significance as well.

It has been demonstrated previously that the EUSES model may well provide a reasonably realistic insight into the multi-route exposure pattern of chemicals, provided that the assumed emission pattern of the substances under study is also realistic [10]. Although in the previous report [10] much less substances were studied than in the present one it clearly indicated that for volatile substances inhalation is the paramount route of exposure, while for less volatile substances oral exposure is more important.

Table 4. Comparison between multi-route exposure patterns under the assumptions: a) concentration in groundwater equals $MPC_{water,eco}$ (italics) or b) concentration in groundwater is equal to 0 mg/l (bold).

| substance | percentage of Estimated Average Total Daily Exposure (EATDE) | | | | | | | | EATDE ($\mu\text{g}/\text{kg bw}/\text{d}$) |
|-----------------------|--|-----------------------|---------------------|----------------------|---------------------|---------------------|-----------------------|-------------------------|--|
| | drinking water | fish | leaf crops | root crops | meat | milk | air | | |
| 1,1-dichloroethylene | 62.78 50.85 | 2.62 4.25 | 0.00 0.00 | 6.85 0.00 | 0.00 0.00 | 0.00 0.01 | 27.74 44.89 | 154.67 95.57 | |
| ethylene | 90.54 93.17 | 0.91 1.87 | 0.00 0.00 | 6.15 0.00 | 0.00 0.00 | 0.01 0.01 | 2.40 4.95 | 268.38 129.87 | |
| ethylene oxide | 74.98 64.46 | 0.58 1.00 | 0.00 0.00 | 4.34 0.00 | 0.00 0.00 | 0.01 0.01 | 20.09 34.54 | 3.20 1.86 | |
| 1,1,2-trichloroethane | 85.16 94.21 | 3.77 4.17 | 0.01 0.00 | 9.61 0.00 | 0.00 0.00 | 0.01 0.01 | 1.45 1.61 | 265.40 239.89 | |
| 1,2-dichloroethylene | 83.60 85.30 | 3.50 7.14 | 0.00 0.00 | 9.18 0.00 | 0.00 0.00 | 0.00 0.01 | 3.70 7.55 | 208.12 102.11 | |
| benzo(a)pyrene | 0.18 0.16 | 22.83 84.87 | 1.45 5.29 | 72.90 0.00 | 1.33 4.84 | 1.33 4.84 | 0.00 0.00 | 0.81 0.22 | |
| ethylbenzene | 30.89 27.56 | 16.09 28.76 | 0.06 0.11 | 28.59 0.00 | 0.00 0.01 | 0.00 0.01 | 24.36 43.56 | 34.31 19.19 | |
| monochlorobenzene | 42.70 39.14 | 13.68 25.05 | 0.04 0.07 | 24.06 0.00 | 0.00 0.00 | 0.00 0.00 | 19.51 35.73 | 46.13 25.19 | |

5.3 Comparison with results of IV-project

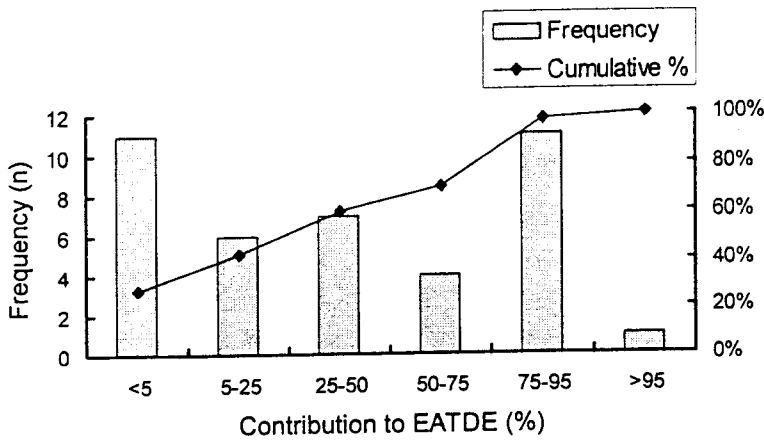
For the determination of the final integrated IV, ecotoxicological and human toxicological limit values were compared. For metals and PAHs the ECOTOX SCC appeared to be the most stringent criterion, while for other organic substances the overall balance between HUM-TOX SCC vs. ECOTOX SCC was 35 to 20 [19]. For the 27 volatile substances also studied in IEQS framework the balance was even more skewed: 22 for which HUM-TOX SCC was the most stringent criterion vs. 5 for which ECOTOX SCC was most important. (see appendix II)

When comparing human exposure patterns as derived in the present report with those obtained with the CSOIL programme IV-project, several differences in the methodology of derivation are observed:

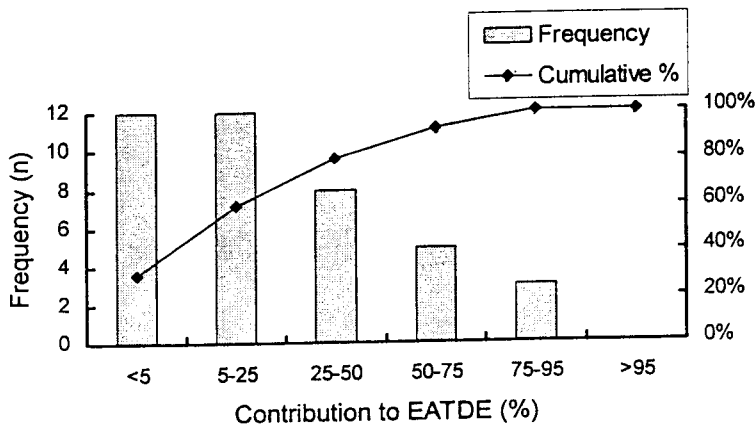
1. several routes in CSOIL are not represented in EUSES, and vice versa. This is for instance the case with inhalation of indoor air (CSOIL +, EUSES -) and with fish or meat consumption (CSOIL-, EUSES +).
2. in CSOIL air contamination, whether outdoor or indoor, is only caused by the local contamination. For substances with low volatility such as PAHs or metals this route will be not very important. In EUSES air contamination is the result from a "distant" emission source. If such a source emits substances such as PAH or metals to air relevant inhalatory exposure of the general population may occur, especially if emitted substances have high inhalatory toxicity.
3. in CSOIL, drinking water contamination is only the result of running of water mains through the contaminated site at which penetration of the pipe walls by the contaminant is assumed. In the present project, the concentration in drinking water is directly related to the $MPC_{\text{water, eco}}$, the assumed level of contamination of the raw drinking water. The assumption for CSOIL is useful in the risk-evaluation of local soil contamination situations, but it cannot be applicable to derivation of harmonised eco-and human toxicological MPCs which have a more generic nature.
4. environmental concentrations (in air and pore water) in CSOIL are entirely dependent on the infinitely lasting concentration of the contaminant at the specific site. In the present study the concentrations in water and soil depend by definition on toxicological criteria, thus having a completely different background.
5. uptake models of soil contaminants by plants are different from the ones in EUSES.
6. CSOIL predicts that ingestion of soil may be an important route of exposure. The calculations in CSOIL take into account the behaviour of children who are assumed to swallow 150 mg soil per day. Given a body weight of 15 kg, the dose of a contaminant, expressed as mg/kg b.w./d may be considerable. In the present report only exposure of adults to soil contaminants has been taken into account (50 mg/soil per day, 70 kg of body weight).

Among others, these differences in methodology (and especially no 6) may well be responsible for the fact that in the IEQS-framework (this report) human exposure through soil ingestion may be of no relevance while in IV-framework it is.

(a) air



(b) Drinking Water



(c) diet

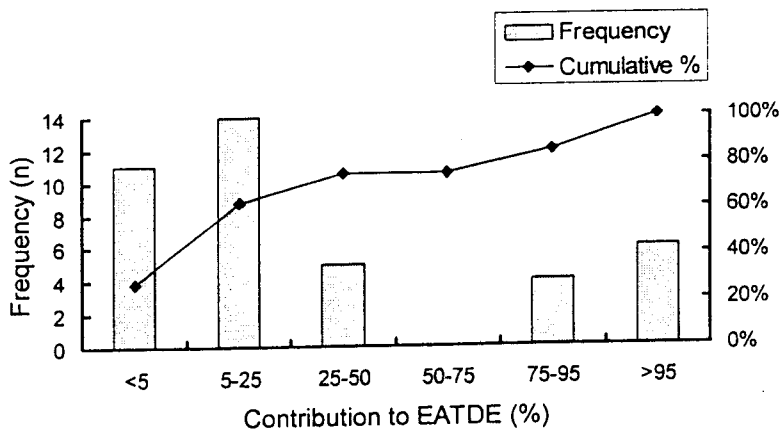


Figure 2. Frequency and cumulative distribution of the relative contribution of exposure via air, drinking water and diet to Estimated Average Total Daily Exposure (EATDE).

Conversely, in this report exposure via drinking water and diet constituents (usually vegetables) is important whereas in IV context most important routes are inhalation of indoor air and vegetables but not drinking water.

5.4 Discussion on confidence in exposure estimates and patterns

The model output of the calculation the EATDEs depends strongly on the height of the MPCs derived for air, water, soil and sediment, which were entered into the EUSES model as predicted regional environmental concentrations (regional PECs). These concentrations were the starting points for the calculations yielding the EATDEs. Similar to the EATDEs the exposure patterns are highly influenced by the environmental concentrations (in this case the MPC_{ecoS} and $MPC_{air, human}$) and other values or actual concentrations may well result in different patterns.

5.4.1 exposure via air

The model used to estimate human exposure can be characterised as being very direct (i.e. only a few calculations and additional assumptions were necessary to arrive at EATDEs). This is especially the case for inhalatory exposure in which the only parameters are concentration in air, respiration rate, body weight and bioavailability. Therefore, the estimates of the contribution via the inhalation route can be expected to be fairly accurate, if concentrations in air would ever reach the MPC_{air} . Thus, for those substances for which inhalation is the main route of exposure, the EATDEs are probably also fairly accurately predicted.

5.4.2 exposure via drinking water

For exposure via drinking water, it has been made plausible that standard procedures to prepare drinking water from groundwater are a rather ineffective means to prevent human exposure via this route [20, 44]. It is conceivable, however, that if groundwater is aerated before distribution, as is fairly often the case, for volatile substances a substantial reduction in the concentration in the drinking water may be reached as a profitable side-effect (personal communication J. Versteegh, RIVM-LWD, 1998). Anyway, the EUSES-model chooses the highest concentration in either unpurified groundwater or purified surface water as the concentration of a contaminant in drinking water. This implicates that at least for less volatile substances the assumptions in EUSES can be characterised as "realistic worst-case", indicating that for such substances exposures as listed in table 1 can occur, if the concentrations in water would ever be equal to the MPCs.

5.4.3 exposure via food

Estimation of human exposure to dietary constituents depends not only on assumptions with respect to human consumption. Uptake and accumulation of environmental contaminants by soil, cattle and fish are equally important, for these processes determine the concentrations of the contaminants in the human diet. The models predicting the concentrations in human food are less direct than those predicting human exposure to air or drinking water contaminants. They rely on QSARs which are "driven" by physico-chemical constants such as K_{ow} and H_c . K_{ow} is an important parameter in the estimation of uptake and accumulation in plants (crops)

and animals (meat/milk, fish), while both K_{ow} and Henry's law constant are relevant for evaporation of substances from plant leaves. The model used to estimate concentration in root crops is believed to perform sufficiently, while concentrations in fish, meat dairy and leaf crops are less accurately predicted [20]. It can thus be assumed that estimates of exposure via root crops are fairly accurate, while exposure estimates via the other dietary constituents are less reliable. These limitations in reliability implicate that for substances for which these routes are predicted to be most important the EATDE may well be over- or underestimated. Moreover, their actual exposure patterns may deviate from the model-predicted ones.

In conclusion: for those chemicals for which either air, water or root crops or a combination of these were the major routes of exposure, EATDEs are probably not entirely unrealistic. For those for which fish or leaf crops were the most important routes, EATDEs are much less reliable. Routes via meat or milk were for all but one (hexachlorobenzene) substances unimportant, but the exposure estimates via these two routes probably have limited accuracy.

It must be noted here that the EATDEs and the exposure patterns mentioned in this report were based on the assumption that in all environmental compartments the MPC_{ecoS} and $MPC_{air, human}$ were simultaneously reached. Although such a situation is theoretically possible, it is probably not very likely to occur. Nevertheless, for the IEQS project it is a prerequisite that these concentrations can occur simultaneously without causing unacceptable exposure of humans and wild-life. So the basic assumption mentioned in the first lines of this paragraph is a matter of definition rather than a description of an actual situation.

Some insight in the influence of both the (nature of the) mathematical model and the "IEQS assumption/definition" (see above paragraph) can be obtained when the exposure patterns as determined by the CSOIL model are compared with those generated by EUSES in the present context. One of the first differences is the fact that for soil contamination sites, ingestion of soil is a very important route of exposure, at least for metals and non-volatile substances. In the present report ingestion via soil was highest for benzo(a)pyrene and even for this substance this route contributed for only 0.08% to the total exposure. Other differences are the fact that for soil contaminants inhalation of indoor air can be important, depending on the substance volatility. This exposure route has not been not incorporated in the EUSES model. The results of the EUSES calculations predict that exposure via drinking water may be important, while in IV-context exposure via drinking water is hardly relevant.

6. Final conclusions and recommendations

The results of this study show that under the assumption that if environmental concentrations were ever equal to the MPCs (for water sediment, soil (eco) and air (human)) derived for the individual substances, for most of the chemicals under study the MPR for humans would be exceeded. In fact only for 7 substances (benzo(a)-pyrene, 1,2-dichloropropane, 1,2-dichloropropane, toluene, ethylene, ethylbenzene and 3-chloropropene) the MPR will not be exceeded. For 9 chemicals the MPR will be exceeded by a factor of 1 to 10, for 21 substances by a factor of 10 to 100 and for four substances (1,2,3,5-tetrachlorobenzene, 1,3,5-tetrachlorobenzene, 1,4-dichlorobenzene and hexachlorobenzene) even by a factor > 100. Whether this immediately indicates a health risk resulting from long-term exposure of the general population remains questionable. For this uncertainty two reasons can be given:

- The EATDEs, which are based on the current sets of MPCs, may be fairly reliable. However, it should be noted that the assumption that in all compartments the MPCs will ever simultaneously be reached is probably very “extreme”.
- For about half of the number of substances MPRs and $MPC_{\text{air, human}}$ s have been derived from a more or less incomplete data set, because of which high uncertainty factors had to be applied. It can thus be anticipated that for some or may be all of these cases the derived MPCs or MPRs are over-conservative. This means that if exposure would exceed the MPR, for such a substance a risk need not necessarily be existent.

For a further interpretation in terms of “risk for humans” a more thorough analysis of uncertainties and relevance of model parameters may be advisable. A discussion on the desirability of the primary assumptions (emissions of volatiles to only water, emission of BaP to only to air and all MPCs reached simultaneously) may be advisable, too, because they both lead to maximisation of the EATDEs. Especially the assumption that water is the primary environmental compartment to which emissions occur is an important factor to determine the relevance of the identified routes of exposure for the various chemicals in the present approach. For volatile substances, this assumption may lead to both unrealistic multi-route exposure patterns as well as to over-estimation of the average daily total exposure of humans. At least under this assumption it seems that for most of the volatile chemicals under study, oral exposure may contribute to the total exposure to a considerable degree or even may be the major route of exposure, which seems to be conflicting to what one would expect to occur in real life and which was indicated by previous results [10].

For quite a number of substances insufficient knowledge is available to derive harmonised (= integrated) sets of MPCs and MPRs. Data gaps may either pertain to human criteria (MPR and $MPC_{\text{air, human}}$; e.g. some of the volatiles, PAHs), to methodological draw-backs (e.g. metals), to environmental behaviour (e.g. metals) or to a combination of these. In order to generate final sets of harmonised MPCs for more substances, it is recommended that methodological draw-backs are alleviated, either by fundamental research, leading to better models, or by generation of reliable measured data. This will also contribute to the IV-project. Lack of limit values can in

some cases be compensated for by introduction of higher uncertainty factors. Up to now for volatile substances for which such high uncertainty factors were applied, only preliminary sets of MPCs have been derived and their use in policy making has not been encouraged [7]. Consequently, these preliminary sets of have not been incorporated into environmental policy as IEQS.

From the results in the present report it can be concluded that even for volatile substances it is insufficient to focus only on inhalatory exposure as was previously done in the IEQS-project (see ref. 7). Weighing of whole body exposure estimates such as EATDE against MPR should be an integral part of the harmonisation procedure. For less volatile substances such as benzo(a)pyrene this seems to be rather obvious.

The results obtained in the present report are not equivalent to the results generated in IV-context due to methodological differences. However, the latter data also indicate that for derivation of IEQSs both human and ecotoxicological criteria should be taken into account.

A possible way to accomplish such a weighing is by starting the integration procedure with EUSES at the level of emissions. At least for organic substances (whether volatile or not) estimations of human daily exposure can be generated either based on realistic emission patterns (cf. ref. 10) or based on the default emission patterns which are part of the EUSES programme [20]. Simply by increasing or decreasing the total emission a point can be reached at which:

- 1) for none of the relevant environmental compartments the contaminant concentration is above the MPC (eco or human)

and simultaneously

- 2) the EATDE is less than the MPR.

Whether calculations should be based on realistic or on default emission patterns is a matter of choice. For certain substances actual emission patterns deviate from the EUSES default patterns to a large extent, which may strongly affect the validity of the model results if defaults are applied. For instance, BaP is largely emitted to air [27], while according to EUSES defaults, emission is for 91 % to water and for 7 % to soil. Although time-consuming it may be profitable in the end to use as many real-life emission pattern data as possible.

Further choices with respect to the development of IEQSs should be how to deal with uncertainties in or lack of physico-chemical data and limit values and what to do with substances for which the present models are unsuitable (e.g. human exposure to metals via fish, meat or vegetables).

It seemed attractive to approach these substances analogous to the derivation of Intervention Values for Soil Clean-up, for which it can be demonstrated that the human toxicological criterion is not the one on which the final (proposed) Intervention Value is based. Similarly one might assume that for the IEQS-project, for these

substances the human toxicological criteria might be left out of consideration. However, because IEQS are meant to be generic standards, while IVs are site-specific standards and because of differences between IV and IEQS in the underlying assumptions, such a “methodological extrapolation” appears not justified. Especially for less volatile substances with high inhalatory toxicity, which are emitted to air to a large extent (viz. PAHs, certain metals) extrapolation from CSOIL with respect to the relevance of ecotoxicological versus human toxicological criteria is inappropriate, as yet.

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Appendix I

Table 5: Volatile Substances: overview physico-chemical parameters

| substance | Mw ^a g/mol | Sol ^b mg/l | log K _{ow} ^a | Vp ^a kPa | Hc ^a Pa/m ³ .mol | Kp _{soil} ^a l/kg |
|----------------------------|--------------------------|--------------------------|----------------------------------|------------------------|--|---|
| harmonised | | | | | | |
| 1,1,1- trichloroethane | 133.41 | 4400 | 2.49 | 13.3 | 980 | 3.3 |
| 1,1-dichloroethylene | 96.94 | 2500 ^[1] | 1.86 | 72.4 | 1560 | 3.6 |
| 1,2-dichloroethane | 98.96 | 8690 | 1.48 | 8.53 | 120 | 2.1 |
| 1,2-dichloropropane | 112.97 | 2700 | 1.99 | 6 | 120 | 2.4 |
| 1,3- dichloropropene | 110.97 | 2700 | 1.76 | 4.5 | 70 | 2.9 |
| 2-chloro-1,3-butadiene | 88.5 | | 2.16 | 23.1 | 200 | 7.2 |
| 3-chloropropene | 76.53 | 100 | 1.45 | 38 | 280 | 1.4 |
| acrylonitrile | 53.06 | 73500 | 0.25 | 13.3 | 4 | 0.08 |
| benzene | 78.11 | 1710 | 2.19 | 12.7 | 330 | 4 |
| dichloromethane | 84.93 | 20000 | 1.25 | 46.5 | 90 | 1.8 |
| ethylene | 28.05 | 131 | 1.13 | 4040 | 7230 | 0.67 |
| ethylene oxide | 44.05 | miscible | - 0.3 | 146 | 29800 | 0.02 |
| styrene | 104.15 | 280 ^[1] | 2.95 | 0.6 | 420 | 45 |
| tetrachloroethylene | 165.82 | 150 | 3.4 | 1.87 | 860 | 12 |
| tetrachloromethane | 153.82 | 800 | 2.83 | 11.9 | 1500 | 34 |
| toluene | 92 | 470 | 2.79 | 2.93 | 390 | 5.7 |
| trichloroethylene | 131.39 | 1100 ^[1] | 2.42 | 7.71 | 350 | 5.5 |
| trichloromethane | 119.38 | 8000 | 1.97 | 21.3 | 170 | 3.2 |
| vinylchloride | 62.5 | 1100 | 1.52 | 33.7 | 1520 | 1.7 |
| preliminary | | | | | | |
| 1,1,2,2-tetrachloroethane | 167.85 | 2900 | 2.39 | 0.793 | 30 | 4.2 |
| 1,1,2-trichloroethane | 133.39 | 4400 ^[2] | 1.89 | 3 | 40 | 4.9 |
| 1,1-dichloroethane | 98.96 | 5500 | 1.79 | 30.2 | 370 | 3.1 |
| 1,2,3,4-tetrachlorobenzene | 215.88 | 3.5 | 4.64 | 0.005 | 30 | 300 |
| 1,2,3,5-tetrachlorobenzene | 215.88 | 2.4 | 4.66 | 0.01 | 50 | 300 |
| 1,2,3-trichlorobenzene | 181.43 | 12 | 4.14 | 0.028 | 130 | 100 |
| 1,2,4,5-tetrachlorobenzene | 215.88 | 0.3 | 4.6 | 0.0007 | 40 | 300 |
| 1,2,4-trichlorobenzene | 181.43 | 19 | 4.05 | 0.061 | 130 | 100 |
| 1,2-dichlorobenzene | 147.01 | 145 ^[2] | 3.43 | 0.196 | 170 | 22 |
| 1,2-dichloroethylene | 96.94 | 800 | 1.86 | 31.5 | 170 | 3.6 |
| 1,2-xylene | 106.16 | 142 ^[3] | 3.12 | 0.667 | 290 | 66 |
| 1,3-dichlorobenzene | 147.01 | 111 ^[2] | 3.53 | 0.307 | 220 | 22 |
| 1,3-dichloropropane | 112.97 | 2870 ^[4] | 2 | 6 | 180 | 5 |
| 1,3-xylene | 106.16 | 147 ^[3] | 3.2 | 0.8 | 420 | 16 |
| 1,4-dichlorobenzene | 147.01 | 70 ^[2] | 3.44 | 0.09 | 210 | 22 |
| 1,4-xylene | 106.16 | 185 ^[3] | 3.15 | 0.867 | 430 | 16 |
| 2,3-dichloropropene | 110.97 | 2150 | 2.04 | 7.1 | 120 | 5.5 |
| 2-chlorotoluene | 126.58 | 47 ^[1] | 3.32 | 0.36 | 490 | 105 |
| 3-chlorotoluene | 126.58 | 114 ^[1] | 3.28 | 0.36 | 400 | 95 |
| 4-chlorotoluene | 126.58 | 150 ^[1] | 3.33 | 0.31 | 490 | 110 |

| substance | Mw ^a g/mol | Sol ^b mg/l | log K _{ow} ^a | Vp ^a kPa | Hc ^a Pa/m ³ .mol | Kp _{soil} ^a l/kg |
|--------------------|--------------------------|--------------------------|----------------------------------|------------------------|--|---|
| ethylbenzene | 106.16 | 152 | 3.15 | 0.933 | 330 | 8.3 |
| hexachlorobenzene | 284.8 | 0.005 ^[2] | 5.73 | 1.5e-6 | 20 | 550 |
| hexachloroethane | 236.72 | 50 | 4.14 | 0.028 | 600 | 200 |
| monochlorobenzene | 112.57 | 500 | 2.9 | 1.58 | 250 | 11 |
| pentachlorobenzene | 250.32 | 0.24 | 5.18 | 0.0022 | 30 | 400 |
| pentachloroethane | 202.28 | 1145 ^c | 3.63 | 0.453 | 80 | 210 |

a all values in these columns have been taken from Van de Plassche and Bockting [5] unless otherwise stated.

b all values in this column have been taken from Verschuieren [6] unless otherwise stated.

c calculated from Hc, Vp and Mw.

(appendix I)

Table 6: Volatile Substances: overview of Maximum Permissible Concentrations for four environmental compartments and tolerable exposure levels for humans (MPC_{air, human} and MPR).

| substance | MPC ^a | MPC ^a | MPC ^a | MPC ^a | MPR |
|----------------------------|---------------------------------|--------------------|-------------------|---------------------------------|--------------------------|
| | water, eco mg/m ³ | soil, eco mg/kg | sed, eco mg/kg | air, human mg/m ³ | |
| harmonised | | | | | |
| 1,1,1- trichloroethane | 2100 | 6.9 | 6.9 | 4.8 | 80 ^[7] |
| 1,1-dichloroethylene | 3400 | 12 | 12 | 0.2 | 3 ^{f, [8]} |
| 1,2-dichloroethane | 700 | 1.5 | 1.5 | 0.1 | 14 ^{[9], rtr} |
| 1,2-dichloropropane | 76 | 4.2 | 0.18 | 0.012 | 14 ^{b, [10]} |
| 1,3- dichloropropene | 8 | 0.023 | 0.023 | 0.04 | 67 ^{b, [11]} |
| 2-chloro-1,3-butadiene | | | | 0.001 | |
| 3-chloropropene | 3.4 | 0.0048 | 0.0048 | 0.074 | 16.9 ^{c, rtr} |
| acrylonitrile | 7.6 | 0.00068 | 0.00068 | 0.01 | 0.1 ^[7] |
| benzene | 240 | 0.95 | 0.95 | 0.03 | 4.3 ^{[12], rtr} |
| dichloromethane | 20000 | 36 | 36 | 1.7 | 60 ^[9] |
| ethylene | 8500 | 5.8 | 5.8 | 30 ^d | 6400 ^{c, rtr} |
| ethylene oxide | 84 | 0.0021 | 0.0021 | 0.003 | 0.64 ^{c, rtr} |
| styrene | 570 | 25 | 25 | 0.8 | 77 ^[9] |
| tetrachloroethylene | 330 | 0.16 | 4 | 2.5 | 16 ^[9] |
| tetrachloromethane | 1100 | 37 | 37 | 0.06 | 4 ^[9] |
| toluene | 730 | 1.4 | 4.2 | 0.3 | 430 ^{[9], rtr} |
| trichloroethylene | 2400 | 13 | 13 | 5 | 540 ^{[9], rtr} |
| trichloromethane | 590 | 1.9 | 1.9 | 0.1 | 30 ^[9] |
| vinylchloride | 820 | 1.4 | 1.4 | 0.1 | 3.51 ^[9] |
| preliminary | | | | | |
| 1,1,2,2-tetrachloroethane | 3300 | 14 | 14 | 0.0004 | 3 ^{b, [13]} |
| 1,1,2-trichloroethane | 7900 | 39 | 39 | 0.018 | 4 ^{f, [8]} |
| 1,1-dichloroethane | 700 | 1.5 | 1.5 | 0.37 | 80 ^{[7], rtr} |
| 1,2,3,4-tetrachlorobenzene | 24 | 0.072 | 7.2 | 0.0016 | 0.5 ^[9] |
| 1,2,3,5-tetrachlorobenzene | 24 | 0.072 | 7.2 | 0.0016 | 0.5 ^[9] |
| 1,2,3-trichlorobenzene | 67 | 0.24 | 6.7 | 0.004 | 0.5 ^[9] |
| 1,2,4,5-tetrachlorobenzene | 24 | 0.072 | 7.2 | 0.0016 | 0.5 ^[9] |
| 1,2,4-trichlorobenzene | 67 | 0.24 | 6.7 | 0.004 | 0.5 ^[9] |
| 1,2-dichlorobenzene | 250 | 0.4 | 5.5 | 0.06 | 0.5 ^[9] |
| 1,2-dichloroethylene | 6100 | 22 | 22 | 0.036 | 6 ^{e, [7]} |
| 1,2-xylene | 380 | 14 | 14 | 0.34 | 10 ^[9] |
| 1,3,5-trichlorobenzene | 67 | 0.24 | 6.7 | 0.004 | 0.5 ^[9] |
| 1,3-dichlorobenzene | 250 | 0.4 | 5.5 | | 0.5 ^[9] |
| 1,3-dichloropropane | 76 | 0.18 | 0.18 | 0.012 | 50 ^{f, [7]} |
| 1,3-xylene | 380 | 14 | 14 | 1 | 10 ^[9] |
| 1,4-dichlorobenzene | 250 | 0.4 | 5.5 | 0.67 | 0.5 ^[9] |
| 1,4-xylene | 380 | 14 | 14 | 1 | 10 ^[9] |
| 2,3-dichloropropane | 8 | 0.044 | 0.044 | | |

| substance | MPC ^a | MPC ^a | MPC ^a | MPC ^a | MPR |
|--------------------|---------------------------------|--------------------|-------------------|---------------------------------|----------------------|
| | water, eco mg/m ³ | soil, eco mg/kg | sed, eco mg/kg | air, human mg/m ³ | |
| 2-chlorotoluene | 310 | 33 | 33 | 0.78 | 20 ^[14] |
| 3-chlorotoluene | 310 | 33 | 33 | | |
| 4-chlorotoluene | 310 | 33 | 33 | | 20 ^[14] |
| ethylbenzene | 370 | 3.1 | 3.1 | 0.039 | 136 ^[9] |
| hexachlorobenzene | 2.4 | 1.3 | 1.3 | 0.0023 | 0.5 ^[9] |
| hexachloroethane | 83 | 17 | 17 | 0.027 | 1 ^{b, [15]} |
| monochlorobenzene | 690 | 7.6 | 7.6 | 0.042 | 0.5 ^[9] |
| pentachlorobenzene | 7.5 | 0.3 | 3 | 0.008 | 0.5 ^[9] |
| pentachloroethane | 230 | 49 | 49 | | |

- a all values in these columns have been taken from Van de Plassche and Bockting [5] unless otherwise stated.
- b For these substances no MPRs were derived by RIVM. However, MPRs or comparable values were derived by other organisations. In order to give a rough impression of a possible risk, these values were used here for MOS calculations. These MPR -values must not be used in policy making before they have been further validated.
- c For 3-chloropropene, ethylene and ethylene oxide an MPR could not be found. The value presented here has been calculated from the MPC_{air, human} (route-to-route extrapolation). In order to give a rough impression of a possible risk, this value was used here for the MOS calculation. The MPR -value must not be used in policy making before it has been further validated.
- d For ethylene an MCP_{air} has not been derived, but for this substance a "limit value in air" of 30 µg/m³ (24 hrs average concentration; see ref. 5) has been set.
- e The given MPR for 1,2-dichloroethylene pertains to the cis-isomer. The MPR for the trans-isomer is about a factor of three higher.
- f The MPRs for 1,1-dichloroethylene and 1,1,2-trichloroethane and the MPC_{air, human} for 1,3-dichloropropane are provisional.
- g. Van de Plassche and Bockting [5] have set the MPC_{eco} for 1,3-dichloropropane equal to those of 1,2-dichloropropane, because they could not perform a calculation with simplebox, due to lack of human data. Because the MPC_{air, human} for 1,3-dichloropropane is still provisional, no adjustment of MPCs would have been carried out. Calculation of the EATDE in the present report is based on the MPC/MPR as presented here.
- rtr Route-to-route extrapolation, assuming a respiration rate of 20 m³/person/day, a body weight of 70 kg and a bioavailability of 100% after oral and 75% after inhalatory exposure.

(appendix 1)

Table 7: *Polycyclic Aromatic Hydrocarbons: physico-chemical data*

| substance | Mw ^a g/mol | Sol ^a mg/l | log K _{ow} ^a | Vp ^a kPa | Hc ^b Pa/m ³ .mol |
|-------------------------|--------------------------|--------------------------|----------------------------------|------------------------|--|
| naphthalene | 128.2 | 31 | 3.30 | 10.4e-3 | 49.8 |
| anthracene | 178.2 | 0.045 | 4.45 | 1e-6 | 4.69 |
| phenanthrene | 178.2 | 1.1 | 4.46 | 2e-7 | 3.81 |
| fluoranthrene | 202.3 | 0.260 | 5.16 | 1.2e-6 | 1.14 |
| benzo(a)anthracene | 228.3 | 0.011 | 5.79 | 2.8e-8 | 0.67 |
| chrysene | 228.3 | 0.0088 | 5.73 | 5.7e-10 | 0.018 |
| benzo(k)fluoranthene | 252.3 | 0.0008 | 6.00 | 5.2e-11 | 0.019 |
| benzo(a)pyrene | 252.3 | 0.0038 | 5.97 | 7e-10 | 0.056 |
| benzo(ghi)perylene | 268.4 | 0.00026 | 6.63 | 2.6e-12 | 0.003 |
| indeno (1,2,3-cd)pyrene | 276 | 0.00005 | 6.4 | 2.6e-12 | 0.017 |

a all values in these columns have been taken from Kalf *et al.* [16] unless otherwise stated.

b all values in this column were re-calculated from Kalf *et al.* [16], who give dimensionless Hc.

The re-calculation is as follows: $Hc (Pa/m^3 \cdot mol) = Hc (dimless) \times RT$ with $R = 8.314 J/mol.K$ and $T = 288K$.

(appendix 1)

Table 8: *Polycyclic Aromatic Hydrocarbons: toxicological criteria*

| substance | CCa ^a | MPC ^b | MPC ^b | MPC ^b | MPC _{air} | MPR |
|-------------------------|-------------------|---------------------------------|--------------------|-------------------|--------------------|---------------------|
| | µg/m ³ | water, eco mg/m ³ | soil, eco mg/kg | sed, eco mg/kg | mg/m ³ | µg/kg b.w./d |
| naphthalene | 140 | 1.2 | 0.14 | 0.14 | | 50 ^[12] |
| anthracene | 8.58 | 0.07 | 0.12 | 0.12 | | 50 ^[12] |
| phenanthrene | 33.4 | 0.3 | 0.51 | 0.51 | | 20 ^c |
| fluoranthrene | 13.1 | 0.3 | 2.6 | 2.6 | | 20 ^c |
| benzo(a)anthracene | 0.218 | 0.01 | 0.25 | 0.36 | | 20 ^c |
| chrysene | 1.32 | 0.34 | 10.7 | 10.7 | | 2 ^c |
| benzo(k)fluoranthene | 0.240 | 0.04 | 2.4 | 2.4 | | 20 ^c |
| benzo(a)pyrene | 0.032 | 0.05 | 0.26 | 2.7 | 1e-6 ^d | 2 to 4 ^c |
| benzo(ghi)perylene | 0.703 | 0.03 | 7.5 | 7.5 | | 20 ^c |
| indeno (1,2,3-cd)pyrene | 0.577 | 0.04 | 5.9 | 5.9 | | 20 ^c |

a CCa: Critical Concentration in air. Derivation of data has been given in Kalf *et al* [16], but in that reference three data are mistyped. Correct values have been presented in Traas *et al* [17].

b all data in these columns have been taken from [16]

c Only for benzo(a)pyrene sufficient data were available to derive an MPR which ranged from 2 to 4 µg/kg b.w./d. The MPRs of the other PAHs were derived from the lower limit of the MPR of benzo(a)pyrene using a relative potency factor (to benzo(a)pyrene); cf ref. 9.

d Slooff *et al.* [18] did not provide an MPC_{air} for individual PAHs. Only a "group" MPC was derived for which benzo(a)pyrene was used as a guide substance. The PAH-mixture in air, resulting from combustion of coal is thought to represent a risk on cancer of 1 per 10⁴ if the benzo(a)pyrene concentration is 1 ng/m³.

(appendix 1)

Table 9: *Metals: physico-chemical constants*

| Element | log Kow ^a | Vp ^a kPa | Mw [19] g/mol | Sol ^a mg/l | Hc ^a Pa.m ³ .mol ⁻¹ . |
|------------------------------------|----------------------|------------------------|---------------------|--------------------------|---|
| As | 10 | 1 e -33 | 74.92 | c | c |
| Ba | 10 | 1 e -33 | 137.33 | c | c |
| Be | 10 | 1 e -33 | 9.01 | c | c |
| Cd | 10 | 1 e -33 | 112.41 | c | c |
| Co | 10 | 1 e -33 | 58.93 | c | c |
| Cr (III) | 10 | 1 e -33 | 52 | c | c |
| Cr (VI) | 10 | 1 e -33 | 52 | c | c |
| Cu | 10 | 1 e -33 | 63.55 | c | c |
| Hg | 10 | 2 e-3 [20] | 200.59 | | 0.03 ^d |
| Hg-(CH ₃) ₂ | | | 230.67 ^b | | |
| Mo | 10 | 1 e -33 | 95.94 | c | c |
| Ni (inorg) | 10 | 1 e -33 | 58.69 | c | c |
| Pb | 10 | 1 e -33 | 207.2 | c | c |
| Sb | 10 | 1 e -33 | 121.75 | c | c |
| Se | 10 | 1 e -33 | 78.96 | c | c |
| Sn | 10 | 1 e -33 | 118.69 | c | c |
| Tl | 10 | 1 e -33 | 204.38 | c | c |
| V | 10 | 1 e -33 | 50.94 | c | c |
| Zn | 10 | 1 e -33 | 65.38 | c | c |

a All values in these columns are arbitrarily set in order to enable SimpleBox and EUSES calculations. The reasons for their choice have been given in Traas *et al.* [17] and in Crommentuijn *et al.* [21].

b calculated

c Traas *et al.* [17] and Crommentuijn *et al.* [21] did not provide Sol and Hc values for metals. These authors used the air-water partition coefficient, instead. For all metals except for Hg this coefficient was set at 10^{-10} .

d Hc calculated from $K_{\text{air-water}}$ (1.3 e-5) by multiplication by 2390 (see note b in table 7).

(appendix 1)

Table 10: **Metals: ecotoxicological MPCs**

| element | MPC _{soil} ^a mg/kg dwt ^c | MPC _{sed} ^a mg/kg dwt ^c | MPC _{water} ^{a,b} µg/l | CCa ^a µg/m ³ |
|------------------------------------|--|---|---|---------------------------------------|
| As | 34 | 190 | 25 | 1.8 |
| Ba | 165 | 300 | 220 | 28 |
| Be | 1.1 | 1.2 | 0.18 | 0.29 |
| Cd | 1.6 | 30 | 0.42 | 0.075 |
| Co | 33 | 19 | 2.8 | 8.3 |
| Cr (III) and (VI) | 100 ^d | 1720 ^e | 8.7 ^c | 9.2 |
| Cu | 40 | 73 | 1.5 | 0.41 |
| Hg | 2.2 ^d | 26 ^d | 0.24 ^d | 0.09 |
| Hg-(CH ₃) ₂ | 0.67 | 1.4 | 0.02 | 0.03 |
| Mo | 254 | 250 | 290 | 2.9 |
| Ni (inorg) | 38 | 44 | 5.1 | 3.2 |
| Pb | 140 | 4800 | 11 | 0.74 |
| Sb | 3.5 | 19 | 6.5 | 0.41 |
| Se | 0.81 | 2.9 | 5.3 | 0.41 |
| Sn | 53 | 22000 | 18 | 0.28 |
| Tl | 1.3 | 2.6 | 1.6 | 0.08 |
| V | 43 | 56 | 4.3 | 1.4 |
| Zn | 160 | 620 | 9.4 | 10 |

a all data in these columns were taken from Crommentuijn *et al.* [21]; CCa: Critical Concentration in air

b MPC_{water} refer to fresh water

c Dutch "standard soil or sediment" contains 25% lutum and 10% organic matter

d based on data for Cr(III)

e based on data for Cr(VI)

f based on value for methyl mercury

(appendix I)

Table 11: **Metals:** Human toxicological criteria and bioconcentration factors for components of the human diet.

| Metal | MPR μg/kg/d | MPC _{air} , human μg/m ³ | BCF _{plant} ^{a, [22]} | | BCF _{meat} | BCF _{milk} | BCF _{fish} |
|------------|---------------------------|--|---|---------------------|--------------------------|--------------------------|---------------------|
| | | | shoots | roots/tubers | | | |
| As | 2.1 ^[9] | | 0.03 | 0.015 | | | 50 ^b |
| Ba | 20 ^{c, [9]} | | 0.1 | 0.005 | | | |
| Be | 0.5 ^[7] | 0.04 ^[7] | 0.001 | 0.005 | | | |
| Cd | 1 ^[9] | | 0.7 | 0.15 | | | 100 ^b |
| Co | 1.4 ^[9] | | 0.03 | 0.015 | | | |
| Cr (III) | 5 ^[9] | | 0.02 ^d | 0.002 ^d | | | 200 ^b |
| Cr (VI) | 7 e-4 ^{rtr, [9]} | 2.5 e-3 ^[20] | 0.02 ^d | 0.002 ^d | | | |
| Cu | 140 ^[9] | | 0.1 | 0.1 | | | 1000 ^b |
| Hg | 0.61 ^{e, [9]} | | 0.03 ^d | 0.015 ^d | | | 1000 ^b |
| methyl-Hg | 0.4 ^{e, [9]} | | 0.03 ^d | 0.015 ^d | | | f |
| Mo | 10 ^[9] | | 0.3 | 0.015 | | | |
| Ni (inorg) | 50 ^[9] | | 0.1 | 0.07 | | | 200 ^b |
| Pb | 3.6 ^[9] | | 0.03 | 0.001 | 0.004 ^{g, [23]} | 0.001 ^{g, [23]} | 5000 ^b |
| Sb | 0.86 ^[7] | | 0.9 | 0.6 | | | |
| Se | 5 ^[8] | | 1 ^h | 1 ^h | | | |
| Sn | 2000 ^[9] | | 0.03 | 0.015 | | | |
| Tl | 0.2 ^[8] | | 3 ^[24] | 3 ^[24] | | | |
| V | 2 ^[8] | 1 ⁽⁷⁾ | 0.3 ^[24] | 0.3 ^[24] | | | |
| Zn | 1000 ^[9] | | 0.4 | 0.1 | | | 10000 ^b |

a Data are in mg/kg dry-weight_{plant}/mg/kg dry-weight_{soil}.

b based on personal communication between RIZA and Bockting as reported in Bockting *et al.* [25].

Given BCFs are based on fish dry-weight (l/kg dwt). For calculation of concentration in fish C_{fi}:
 $C_{fi} = C_{wa} \times BCF_{fi} \times fdw_{fi}$. $fdw_{fi} = 0.1 \text{ kg}_{dw}/\text{kg}_{fw}$. For missing data, additional information has been requested at RIZA (C. van der Guchte, 1997). Recent data show that the bioaccumulation factor in fish is fairly reliable for Cd, but that the bioaccumulation of Hg is probably a factor of 10 (lean fish) to 50 (fatty fish) too low. For the other metals data are too scanty to derive bioaccumulation factors.

c Soluble Barium; For total Ba the MPR = $20 \times [\text{Total}]/[\text{dissolved}] \text{ μg/kg/d}$.

d speciation in soil not further defined

e exposure tot total Hg, however, contribution of methyl-Hg must not be higher than indicated under the latter compound.

f Bioaccumulation of this substance in fish may be estimated from the Kow. However, if calculations are carried out with the concentration of Hg-(CH₃)₂ as starting point, the estimate of the concentration in fish appears to be too low. A better estimate is obtained when calculations are based on total Hg. Possibly, total Hg is bioavailable as Hg-(CH₃)₂ (personal communication, R. Luttik, 1997) This is further substantiated by the finding that virtually all Hg in aquatic animals occurs as methyl mercury [26].

g This values are in mg/kg fresh product/mg/kg feed. The validity of these values is unclear.

h BCF_{plant} was taken from CSOIL version 1.0 [27]. In the newer version (cf. ref. 24) for Se no BCF_{plant} was given

rtr calculated via route-to-route extrapolation from MPC_{air, human} for procedure see under appendix I, table 6

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Appendix II

Overview of human and ecotoxicological Serious soil Contamination Concentrations and finally proposed integrated intervention values.

| substance | HUM-TOX | ECOTOX | integrated | comment |
|--|------------------|--|---------------------|------------------|
| | SCC ^a | SCC ^a | intervention | |
| | mg/kg soil | mg/kg soil | value ^b | |
| | | | mg/kg soil | |
| 1,1,1- trichloroethane | 15 | 88 | 15 ^[1] | |
| 1,1-dichloroethylene | 0.216 | 130 | 0.22 ^[2] | |
| 1,2-dichloroethane | 3.9 | 60 | 4 ^[3] | |
| 1,2-dichloropropane | 1.81 | 125 | 1.8 ^[2] | both isomers |
| 1,3- dichloropropene | | | | no value derived |
| 2-chloro-1,3-butadiene | | | | no value derived |
| 3-chloropropene | | | | no value derived |
| acrylonitrile | 0.093 | 1.3 | 0.1 ^[1] | |
| benzene | 1.1 | 25 | 1.1 ^[3] | |
| dichloromethane | 60 | 19 | 19 ^[3] | |
| ethylene | | | | no value derived |
| ethylene oxide | | | | no value derived |
| styrene | 100 | - | 100 ^[3] | |
| tetrachloroethylene | 3.9 | 60 | 4 ^[3] | |
| tetrachloromethane | 0.92 | 60 | 1 ^[3] | |
| toluene | 340 | 130 | 130 ^[3] | |
| trichloroethylene | 300 | 60 | 60 ^[3] | |
| trichloromethane | 8.9 | 60 | 9 ^[3] | |
| vinylchloride | 0.078 | 60 | 0.1 ^[3] | |
| 1,1,2,2-tetrachloroethane | | | | no value derived |
| 1,1,2-trichloroethane | 8.38 | 460 | 8.4 ^[2] | |
| 1,1-dichloroethane | 15 | 42 | 15 ^[3] | |
| tetrachlorobenzene | 17 | 30 | 17 ^[3] | all isomers |
| trichlorobenzene | 8.8 | 30 | 9 ^[3] | all isomers |
| dichlorobenzene | 190 | 30 | 30 ^[3] | all isomers |
| 1,2-dichloroethylene (<i>cis</i>) | 0.51 | 238 | 0.5 ^[1] | |
| 1,2-dichloroethylene (<i>trans</i>) | 0.81 | 238 | 1 ^[1] | |
| xylene | 26 | - | 26 ^[3] | all isomers |
| 1,3-dichloropropane | | see 1,2-dichloropropane ^[2] | | |
| 2,3-dichloropropene | | | | no value derived |
| 2-chlorotoluene | | | | no value derived |
| 3-chlorotoluene | | | | no value derived |
| 4-chlorotoluene | | | | no value derived |
| ethylbenzene | 50 | - | 50 ^[3] | |
| hexachlorobenzene | 25 | 30 | 25 ^[3] | |
| hexachloroethane | | | | no value derived |
| monochlorobenzene | 530 | 30 | 30 ^[3] | |
| pentachlorobenzene | 23 | 30 | 23 ^[3] | |
| pentachloroethane | | | | no value derived |
| naphtalene | 590 | 40 | 40 ^[3] | |
| anthracene | 29000 | 40 | 40 ^[3] | |
| phenanthrene | 630 | 40 | 40 ^[3] | |
| fluoranthrene | 1000 | 40 | 40 ^[3] | |
| benzo(a)anthracene | 11000 | 40 | 40 ^[3] | |

| substance | HUM-TOX SCC ^a | ECOTOX SCC ^a | integrated intervention value ^b | comment |
|------------------------------------|-----------------------------|----------------------------|--|------------------------------------|
| | mg/kg soil | mg/kg soil | mg/kg soil | |
| chrysene | 360 | 40 | 40 ^[3] | |
| benzo(k)fluoranthene | 11000 | 40 | 40 ^[3] | |
| benzo(a)pyrene | 1000 | 40 | 40 ^[3] | |
| benzo(ghi)perylene | 12000 | 40 | 40 ^[3] | |
| indeno (1,2,3-cd)pyrene | 12000 | 40 | 40 ^[3] | |
| As | 680 | 40 | 40 ^[3] | |
| Ba | 4300 | 625 | 625 ^[3] | |
| Be | 233 | 29 | 30 ^[4] | |
| Cd | 35 | 12 | 12 ^[3] | |
| Co | 450 | 240 | 240 ^[3] | |
| Cr (III) | 2250 | 230 | 230 ^[3] | assumed equivalent to Cr- total |
| Cr (VI) | | | | no value derived |
| Cu | 16000 | 190 | 190 ^[3] | |
| Hg | 200 | 10 | 10 ^[3] | |
| Hg-(CH ₃) ₂ | | | | no value derived |
| Mo | 910 | < 480 | 480 ^[3] | |
| Ni (inorg) | 6600 | 210 | 210 ^[3] | |
| Pb | 300 | 290 | 290 ^[3] | |
| Sb | 15.7 | 2890 | 15 ^[4] | |
| Se | 235 | 5 | 5 ^[2] | |
| Sn | 650000 | 910 | 910 ^[2] | updated since ref 3 |
| Tl | 14 | 118 | 14 ^[2] | |
| V | 1000 | 250 | 250 ^[2] | |
| Zn | 56000 | 720 | 720 ^[3] | |

a HUM-TOX SCC, ECOTOX SCC: human and ecotoxicological Serious soil Contamination Concentration, respectively.

b The values in this column are not the final intervention values for soil clean-up, but are the proposals as submitted by RIVM.

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Appendix III

Overview of default values in the EUSES 1.0 and USES 1.0 models and values which have been applied within the setting of the present report. Because the starting point in the evaluations were the various MPCs, defaults which are relevant for emission and distribution are irrelevant within the scope of this report. No defaults have been given for cattle because all defaults were the same within EUSES or USES. No defaults have been given for plants because in EUSES a different model than the one in USES is used to estimate concentrations of environmental contaminants in plant tissues.

| NAME | Value in EUSES 1.0 ^[1] | Value in USES 1.0 ^[2] | applied for report | units |
|--|-----------------------------------|----------------------------------|--------------------|---------------------------------|
| CHARACTERISTICS OF HUMANS | | | | |
| Daily intake of drinking water | 2 | 2 | 2 | l.d ⁻¹ |
| Daily intake of fish | 0.115 | 0.011 | 0.011 | kg.d ⁻¹ |
| Daily intake of leaf crops (incl. fruit and cereals) | 1.2 | 0.349 | 0.349 | kg.d ⁻¹ |
| Daily intake of root crops | 0.384 | 0.129 | 0.129 | kg.d ⁻¹ |
| Daily intake of meat | 0.301 | 0.120 | 0.120 | kg.d ⁻¹ |
| Daily intake of dairy products | 0.561 | 0.378 | 0.378 | kg.d ⁻¹ |
| Inhalation rate for humans | 20 | 20 | 20 | m ³ .d ⁻¹ |
| Bioavailability for oral uptake | 1 | 1 | 1 | - |
| Bioavailability for inhalation | 0.75 | 0.75 | 0.75 | - |
| Bodyweight of the human considered | 70 | 70 | 70 | kg |

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