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The evaluation of the equilibrium partitioning method using sensitivity distributions of species in water and soil or sediment.

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Abstract

The equilibrium partitioning method (EqP-method) can be used to derive environmental quality standards for soil or sediment, from aquatic toxicity data and partitioning coefficients. The validity of the use of the EqP-method for this purpose was studied by the comparison of aquatic with terrestrial toxicity data. For 12 organic substances and for 8 metals sufficient data were available in the literature to make this comparison. For copper, chlorpyrifos, atrazine and for the effect of pentachlorophenol or cadmium on soil processes, the terrestrial toxicity data were significantly higher compared to the aquatic toxicity data but for 2,4,6-trichlorophenol, trichloroethene, chromium III, arsenic and lead they were lower. Some of these statistically significant differences might be attributed to the selection of the sorption constants, but in the case of chlorpyrifos, trichloroethene and chloroform this was not the case. For these compounds the differences might be attributed to the selection of soil or sediment toxicity tests. These significant differences indicate that the EqP-method can give a significant over-or underestimation.

The EqP-method is used to estimate Hazardous Concentration 5% (HC5) values for soil or sediment using aquatic toxicity data. These HC5 values were in 5% of the cases more than a factor 20 higher than the corresponding HC5 values that were derived directly using toxicity tests with soil organisms for the 12 organic substances and 8 metals.

Recommendations are given for the use of the EqP-method for setting soil quality guidelines when only a very limited number of terrestrial toxicity data are available.

Samenvatting

De evenwicht partitie methode (EqP-methode) kan worden gebruikt om milieukwaliteitsnormen (zoals het Maximaal Toelaatbaar Risiconiveau of de interventiewaarde) voor bodem of sediment af te leiden uit aquatische toxiciteitsgegevens en een bodem/water of sediment/water partitiecoëfficiënt. De validiteit van het gebruik van de EpP-methode voor dit doel kan bestudeerd worden door aquatische toxiciteitsdata te vergelijken met terrestrische. Voor 12 organische stoffen en voor 8 metalen waren voldoende gegevens in de literatuur beschikbaar om deze vergelijking te maken. De toxiciteits- en sorptie-data voor water en bodem werden gehaald uit de rapporten die worden gebruikt om milieukwaliteitsnormen in Nederland af te leiden. Met behulp van geselecteerde sorptie constanten (uitgedrukt in L/kg) werden de EC50 (Effect Concentratie 50%) of No Observed Effect Concentration (NOEC) waarden (uitgedrukt in µg/L) voor waterorganismen vergeleken met de EC50 of NOEC waarden (uitgedrukt in mg/kg) voor bodemorganismen of bodem processen.

Voor koper, chloorpyrifos, atrazine en voor het effect van pentachloorfenol of cadmium op bodem processen, waren de terrestrische toxiciteitsgegevens (EC50 of NOEC) significant hoger dan de aquatische toxiciteitsgegevens. Voor 2,4,6-trichloorfenol, trichlooretheen, chroom III, arsenicum en lood waren de aquatische toxiciteitsgegevens significant hoger. Sommige van deze statistisch significante verschillen kunnen misschien worden toegeschreven aan de selectie van de sorptie constanten, maar voor chloorpyrifos en trichlooretheen was dit niet het geval. De significant lagere EC50 waarden van chloroform (trichloormethaan) voor processen in het sediment vergeleken met diersoorten in water, kon ook niet verklaard worden door de selectie van de sorptie constante. Voor chloorpyrifos, trichlooretheen en chloroform kunnen deze statistisch significante verschillen misschien worden toegeschreven aan de selectie van de bodem of sediment toxiciteitstesten.

Deze significante verschillen geven aan dat de EqP-methode geen wetenschappelijk gevalideerde methode is om milieukwaliteitsnormen af te leiden maar alleen beschouwd kan worden als een schattingsroutine die een significante over- of onder-schatting kan geven.

De EqP-methode wordt gebruikt om de Hazardous Concentration 5% (HC5) waarden voor bodem of sediment te schatten met behulp van aquatische toxiciteitsgegevens. Deze HC5 waren in 5% van de gevallen meer dan factor 20 hoger dan de overeenkomstige HC5 waarden, die direct werden afgeleid met behulp van toxiciteitstesten met bodemorganismen voor de 12 organische stoffen en 8 metalen. Deze factor 20 geeft aan dat de EqP-methode niet gebruikt kan worden voor een accurate bepaling van bodem of sediment HC5 waarden, maar alleen geschikt is voor een ruwe schatting.

Wanneer een risicobeoordelaar geconfronteerd wordt met een beperkt aantal terrestrische toxiciteitsgegevens en een veel groter aantal aquatische toxiciteitsgegevens, samen met een betrouwbare bodem/water partitiecoëfficiënt. Dan dient er voor een ruwe schatting van de bodem-kwaliteitsnorm een keuze gemaakt te worden tussen het gebruik van de terrestrische data, of het gebruik van de EpP-methode. De aanbevelingen geven gedetailleerde adviezen voor deze keuze, ten einde de vaak erg grote onzekerheid in de schatting van een bodem-kwaliteitsnorm te minimaliseren.

Summary

The equilibrium partitioning method (EqP-method) can be used to derive environmental quality standards (like the Maximum Permissible Concentration or the intervention value) for soil or sediment, from aquatic toxicity data and a soil/water or sediment/water partitioning coefficient. The validity of the use of the EqP-method for this purpose can be studied by the comparison of aquatic with terrestrial toxicity data. For 12 organic substances and for 8 metals sufficient data were available in the literature to make this comparison. The toxicity and sorption data for water and soil were taken from the reports that are used to derive environmental quality standards in the Netherlands. The EC50 (Effect Concentration 50%) or No Observed Effect Concentration (NOEC) values (expressed in µg/L) for water organisms were compared with the EC50 or NOEC values (expressed in mg/kg) for soil organisms or soil processes using selected sorption constants (expressed in L/kg).

For copper, chlorpyrifos, atrazine and for the effect of pentachlorophenol or cadmium on soil processes, the terrestrial toxicity data (EC50 or NOEC) were significantly higher compared to the aquatic toxicity data. For 2,4,6-trichlorophenol, trichloroethene, chromium III, arsenic and lead the aquatic toxicity data were significantly higher. Some of these statistically significant differences might be attributed to the selection of the sorption constants, but in the case of chlorpyrifos and trichloroethene this was not the case. The significantly lower EC50 values of chloroform (trichloromethane) for processes in sediment compared to animal species in water could also not be explained by the selection of the sorption constant. For chlorpyrifos, trichloroethene and chloroform, these significant differences might be attributed to the selection of soil or sediment toxicity tests. These significant differences indicate that the EqP-method is not a scientifically validated method to derive environmental quality standards but can only be regarded as an estimation routine, which can give a significant over-or underestimation.

The EqP-method is used to estimate Hazardous Concentration 5% (HC5) values for soil or sediment using aquatic toxicity data. These HC5 values were in 5% of the cases more than a factor 20 higher than the corresponding HC5 values that were derived directly using toxicity tests with soil organisms for the 12 organic substances and 8 metals. This factor 20 indicates that the EqP-method can not be used for an accurate determination of soil or sediment HC5 values, but is only suited for a rough estimation.

When a risk assessor is confronted with a limited number of terrestrial toxicity data and a much larger number of aquatic toxicity data, together with a reliable soil/water partitioning coefficient. There is a choice between the use of the terrestrial data, or the use of the EqP-method, for a rough estimation of a soil quality standard. The recommendations give detailed advice for this choice in order to minimize the often very large uncertainty in the estimation of a soil quality standard

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Contents

1. Introduction

1.1 The calculation of environmental quality standards from toxicity data

Two environmental quality standards in the Netherlands are the Maximum Permissible Concentration (MPC) and the Target Value (TV). The standards are used to assess the environmental quality of surface water, air, soil and sediment. Results of toxicity tests are important in the process of deriving MPC values for specific pollutants. Each dose effect curve of a toxicity test can be summarized by a dose effect parameter like the NOEC, EC10, or EC50. The EC10 or EC50 are defined as the toxicant concentrations, which give 10% or 50% inhibition. The NOEC is the highest tested concentration that does not show a statistically significant difference with the control test without added toxicant. The NOEC is dependent on the statistical power of the test and on the experimental setup (concentrations tested) [Hoekstra and Van Ewijk, 1993].

In the Netherlands, the MPC of organic pollutants or metals is determined from toxicity data using the following procedure: The aquatic MPC is derived from the EC50 or NOEC values of a number of chronic aquatic toxicity tests with a specific toxicant. When 4 or more NOEC values from 4 or more taxonomic groups are available, a statistical procedure is used: The average, the standard deviation, and the number of the logarithmically transformed NOEC values are used to calculate a toxicant concentration $HC5^{NOEC}$ (Hazardous Concentration 5%). This is the 5th percentile of the NOEC distribution. Below this concentration, at least 95% of the species are assumed to be protected [Van Straalen and Denneman, 1989]. This toxicant concentration is taken as a starting point for setting the MPC. When only a single EC50 is available then the MPC is set equal to the lowest EC50/1000. When more EC50 or NOEC data are available the assessment factor can be lowered from 1000 to 100, 50, 30 or 10 depending on the number of data available. These methods to calculate the MPC were based on the EU-TGD method [Crommentuijn et al., 2000c] and were recently updated [Traas, 2001]. Similar methods are also available to derive terrestrial MPCs from soil toxicity tests using microbial processes, earthworms, plants or arthropods [EC, 1996; Kalf et al., 1999; Traas, 2001].

1.2 The use of the equilibrium partitioning method to estimate the soil and sediment quality guidelines from aquatic toxicity data

In the Netherlands, the environmental quality standards for water, soil, and sediment are harmonized because it is recognized that pollutants distribute between these environmental compartments. For example, polluted soils can result in groundwater pollution or air pollution and polluted water can give rise to sediment pollution and vice versa. The partitioning of a pollutant between water and a solid phase like sediment, soil or suspended solids can be described by a partition coefficient (Kp). Kp is defined as the concentration ratio between the solid and the aqueous phase at equilibrium:

$$Kp = Csolid\ (mg/kg) / Cwater\ (mg/L) \qquad \{1\}$$

The Kp is expressed in L water/kg solids. The solid phase can be sediment, soil or suspended matter. The Kp makes it possible to predict the equilibrium sediment concentration, when the water concentration is known. This is called the equilibrium partitioning method (EqP-method). This method can be used to estimate a soil or sediment MPC, when the aquatic MPC and the Kp are known and it can also be used to harmonize aquatic and terrestrial MPC values [Kalf et al., 1999]. When the EC50 or NOEC from soil or sediment are used to calculate the corresponding water concentrations using equation {1}, these values will be referred to as EqP-transformed values throughout this report.
The EqP-method is used to estimate terrestrial and sediment MPC values from aquatic MPC values, when insufficient soil and sediment toxicity data are available. In the Netherlands most soil and sediment environmental quality standards are derived from the environmental quality standards for water using the EqP-method. Within the Dutch project "Setting Integrated Environmental Quality Standards for Substances" (INS), environmental quality standards were derived for about 180 substances [De Bruijn et al., 1999]. Recently, this data set was updated with more toxicity data [Verbruggen et al., 2001; Lijzen et al., 2001] and more sorption data [Otte et al., 2001]. For the calculation of the MPC in water the statistical extrapolation method was used for approximately one-third of the compounds while in the remainder of the cases the EU-TGD method was used [Crommentuijn et al., 2000b; Crommentuijn et al., 2000c]. For the calculation of the MPC in soil the statistical extrapolation method was used in approximately one-fourth of the cases. The EU-TGD method was used for one-fifth of the cases. While in the remainder of the cases the EqP-method was used to derive the soil MPC from the water MPC. For sediment the EqP-method was used in all cases because of a lack of ecotoxicological data [Crommentuijn et al., 2000c; Di Toro et al., 1991; Verbruggen et al., 2001]. This illustrates that most of the ecotoxicological data referred to aquatic organisms, a minority of the data referred to soil organisms, while for sediment hardly any data were available.

1.3 The evaluation of the equilibrium partitioning method

In an advice of the Technical Commission Soil Protection [TCB, 1994] it was stated that toxicity data from tests with soil and sediment are necessary to determine an MPC for soil and for sediment. When no data are available, it might be possible to estimate these MPC's from the aquatic MPC and partition coefficients using the EqP-method. The Dutch Health Council stated that the EqP-method was only suited for organic, apolar and not very hydrophobic substances and not for metals since the uncertainty factor of the partition coefficients for metals is large. It lies in the order of magnitude of about 1000 [Gezondheidsraad, 1995]. The lack of soil and sediment toxicity data, noticed in these reports in 1995, is still present nowadays [Verbruggen et al., 2001]. This urges legislators to use the EqP-method to estimate soil and sediment MPC values from aquatic toxicity data. The continued use of the EqP-method despite of the above criticism raised questions about the validity of the method for this purpose. In this report, the outcome of the EqP-method is compared with actual measurements reported in the literature. During this comparison a few questions arise. The first question is: Does the application of the EqP-method on aquatic toxicity data give a significant difference with terrestrial toxicity data? The second question is; Can the differences be explained by differences in the reported Kp values? The third question is: How large are these differences? The final question is: How does this affect the setting of soil and sediment quality standards?

2. Methods

2.1 The selection of the equilibrium partition coefficient Kp for organic substances

In general, the Kp is dependent on both the solid phase e.g. the specific soil, sediment, or suspended solids, the water phase (containing salts, dissolved organic matter, chelators and other compounds) and the redox potential and pH of the system. In the case of organic compounds the Kp is often normalized for the concentration of organic carbon in soil and is called the Koc. The Koc is expressed in units of L water/kg organic carbon. The fraction of organic carbon is called foc and is expressed as kg organic carbon/kg soil.

foc*Koc = Kp {2}

The Koc can be determined experimentally or can be estimated from the octanol-water partition coefficient (Kow) using a Quantitative Structure Activity Relationship (QSAR) [Bockting et al., 1993]. The selection of a specific Koc value from the scientific literature is not a trivial one. The variation in the reported Koc values of a single compound for different soils can be several orders of magnitude [MacKay et al., 1997a; MacKay et al., 1997b; MacKay et al., 1997c; Otte et al., 2001].

In this report two sets of partition coefficients have been used. The first set are the Kp values used for the evaluation of the Intervention Values for the first series of compounds by Otte et al. (2001). They also evaluated the existing datasets for Kp values of metals in soil. The available data sets were ranked according to several criteria including the quality of the data, the metal concentration, compatibility with Dutch soil, and experimental set-up. The second data set are the Kp values formerly used within the framework of the project "Setting Integrated Environmental Quality Standards" [De Bruijn et al., 1999] to derive maximum permissible concentrations (MPCs) and negligible concentrations (NCs).

The Kp values evaluated by Otte et al. (2001) are normalized for a standard soil containing 25% clay, 5.8% organic carbon and pH 6. The Kp values from Annex 1 in the INS report [VROM, 1999] where reported for suspended material in standard surface water with 11.6% organic carbon. Which means that foc for standard soil is 0.5 times the foc for standard suspended material. For organic substances it follows that:

Kp standard soil = 0.5 * Kp suspended material {3}

A logarithmic transformation of equation {2} with foc = 0.058 yields:

log Kp standard soil = log Koc - 1.237 {4}

Table 1 (see last page) shows the selected log Kp values for standard soil from Otte et al. (2001). Only the Kp values for chlorpyrifos, chlordane and heptachlor were taken from Annex 1 in the INS report [VROM, 1999] and where normalized for standard soil using equation {3}. In general the differences in the log Kp values for standard soil between both datasets were small for organic substances.

2.2 Selection of the equilibrium partition coefficient Kp for metals

For metals there was a large difference between the Kp values used by Otte et al. (2001) and the Kp values from Annex 1 in the INS report [VROM, 1999]. Table 1 shows the difference between the Kp values used by Otte et al. (2001) which are listed under the column marked "log Kp" and the Kp values for metals from Annex 1 in the INS report [VROM, 1999] which are listed under the column marked "low". The latter Kp values are from limited studies on the sorption to suspended particles instead of sediment [Kalf et al., 1999]. For most metals these values are orders of magnitude higher than the corresponding Kp values in soil. Because of this wide variability, the use of Kp values for the purpose of equilibrium partitioning was not recommended for the derivation of ecotoxicological risk limits for metals in sediment [Verbruggen et al., 2001]. However a modified equilibrium partitioning method was used [Crommentuijn et al., 2000a; Crommentuijn et al., 2000b]. This modified method used empirical sorption coefficients from Dutch rivers and coastal zones, which represent the generic sites for which environmental quality standards were derived.

2.3 The comparison between aquatic toxicity data and terrestrial or sediment toxicity data using the EqP-method

The INS data set [De Bruijn et al., 1999] and the updated data set [Verbruggen et al., 2001], were screened for organic compounds and metals. The chemicals were selected that had sufficient data for a comparison between aquatic and terrestrial toxicity data using the EqP-method with the selected Kp values. Three selection criteria were used; a) More than 3 EC50 or LC50 (Lethal Concentration 50%) values from terrestrial toxicity tests. b) Or more than 3 chronic NOEC values from chronic terrestrial toxicity tests. c) Or more than 3 NOEC values from tests using microbial processes in soil.
The terrestrial EC50 values were compared with the EC50 values from short-term acute aquatic toxicity tests, whereas the terrestrial NOEC values were compared with the NOEC values from long-term chronic aquatic toxicity tests. For the compounds that had sufficient terrestrial toxicity data there were always sufficient aquatic toxicity data present. The LC50 data are combined with the EC50 data, as is done in the INS report [De Bruijn et al., 1999] and summarized here as EC50 values. When more EC50 values for one species are available, the mean of these logarithmically transformed EC50 values was taken as input parameter (this is equal to the logarithm of the geometric mean of these values). For some acute aquatic toxicity tests, the differences in sensitivity could be explained by differences in the size of the test organisms and the duration of the test. In these cases the lowest EC50 value was selected from a number of tests with the same species. The soil toxicity data were normalized to a standard soil with 10% organic matter (5.8% organic carbon) [Verbruggen et al., 2001].

One of the objectives of this study is to test the hypothesis that the species sensitivity distributions of aquatic and terrestrial species do not differ. A simple way to compare both sensitivity distributions is to compare the underlying data. Normally the EqP-method is used to calculate a soil or sediment concentration from a water concentration using equation {1}. For practical reasons we EqP transformed the soil or sediment concentrations (expressed in mg/kg) into their corresponding water concentrations (expressed in µg/L) using equation {1}. This equation can be written in a logarithmic form:

log EC50water = log EC50soil + 3 - log Kp {5}

with the EC50water in µg/L, the EC50soil in mg/kg and the Kp value for standard soil as described in the above paragraph. The constant 3 is used to convert µg to mg. At this stage the terrestrial toxicity tests can be compared with the aquatic toxicity tests since the log EC50 of both tests are now reported in µg/L. The difference between the EqP transformed terrestrial data and the aquatic data can be calculated using equation {5}.

delta1 = log EC50soil + 3 - log Kp - log EC50water {6}

When equation {5} is true delta1 = 0. The same procedure can be performed with NOEC values instead of EC50 values.

2.4 The use of the modified EqP-method for metals

For both sediment and soil, a modified EqP-method can be applied to derive MPCs from those for water when sufficient toxicological data on sediment and soil organisms are not available. It must be noted that originally the EqP-method normalizes concentrations of organic substances in the solid phase to the organic carbon content. For metals and metalloids, the EqP-method was modified because the organic content normalization was not applied, and empirically derived sediment/water and soil/water partition or distribution coefficients were used [Crommentuijn, 2000b].

For the metals cadmium, copper, lead, mercury and zinc there are a large number of aquatic and terrestrial toxicity data available [De Bruijn et al., 1999; Verbruggen et al., 2001]. The terrestrial toxicity data were normalized for a standard soil with 25% clay, 5.8% organic carbon [De Bruijn et al., 1999; Verbruggen et al., 2001]. This makes it possible to calculate EqP-transformed log NOEC values from aquatic and from terrestrial toxicity data for these metals [Otte et al., 2001]. The NOEC values for soil processes or soil organisms (expressed in mg/kg) were EqP-transformed using:

log NOECwater = log NOECsoil + 3 - log Kp(soil/water) {7}

with NOECwater expressed in µg/L, NOECsoil in mg/kg and log Kp(soil/water) in L/kg

2.5 The comparison between the aquatic HC5 value and the terrestrial HC5 value using the EqP-method

In equation {5} and equation {6} the terrestrial and aquatic toxicity data are compared with respect to their average. This average is also called the log HC50 because below this concentration 50% of the species are protected [Van Straalen and Denneman, 1989]. It is of course also interesting to compare the terrestrial and aquatic toxicity data with respect to their standard deviation. This comparison is not performed here because legislators are more interested in the HC5 value, which is derived from the average and the standard deviation of the toxicity data. These HC5 values can be used for setting environmental quality standards (see introduction). The $HC5^{NOEC}$ or the $HC5^{EC50}$ can be calculated using the following formula [Van Straalen and Denneman, 1989]:

$$\text{Log } HC5^{NOEC} = \text{average (log NOEC)} - \text{constant} * \text{SD(log NOEC)} \qquad \{8\}$$

$$\text{Log } HC5^{EC50} = \text{average (log EC50)} - \text{constant} * \text{SD(log EC50)} \qquad \{9\}$$

With SD = standard deviation, and the constant is a statistical extrapolation constant which is dependent on the number of data and the level of statistical confidence one might want to achieve [Van Straalen and Denneman, 1989].

At this stage the impact of the use of the EqP-method, for the estimation of a terrestrial HC5 from an aquatic HC5, can be evaluated using a logarithmic transformation of equation {1}.

$$\text{log HC5water} = \text{log HC5soil} + 3 - \text{log Kp} \qquad \{10\}$$

With HC5water in µg/liter, HC5soil in mg/kg and Kp in liter/kg.

$$\text{delta2} = \text{log HC5soil} + 3 - \text{log Kp} - \text{log HC5water} \qquad \{11\}$$

When delta2 = 0 the EqP-method is accurate, when delta2 = 1 the EqP-method underestimates the terrestrial HC5soil from the aquatic HC5water with a factor 10.

2.6 Statistical analysis

The aquatic and terrestrial log EC50 or NOEC values were compared using a two sample Students t-test assuming unequal variances [Armitage and Berry, 1994]. The null hypothesis states that the means of the aquatic and terrestrial log EC50 or NOEC values differ by log Kp as in equation {5} and {6}. The two-sided probability is calculated to test whether the null hypothesis is correct. When this probability is below 5% the difference between the means of the aquatic and terrestrial log EC50 or NOEC values is statistically significant. For the comparison of the HC5soil with the HC5water using equation {11} 90% confidence levels were calculated using equations {8} and {9} with the extrapolation constants from Aldenberg and Jaworska (2000). When the confidence levels of the EqP transformed HC5soil did not overlap with the confidence levels of the HC5water the statistical probability is less than 1%. When the HC5soil fell outside of the confidence range of the HC5water the statistical probability is less than 5%. The calculations were performed using Microsoft Excel. The mean and standard deviation (n-1) of the distributions are reported.

3. Results and Discussion

3.1 Does the application of the EqP-method on aquatic toxicity data give significant differences with terrestrial toxicity data?

Table 1 (see last page) shows the average (avrg), the standard deviation (SD) and the number of species (N) from the terrestrial Species Sensitivity Distribution (SSD) and the aquatic SSD. The organic substances and metals were selected from the updated INS data set [Verbruggen et al., 2001] except for chlorpyrifos, chlordane and heptachlor which were only present in the original INS data set [De Bruijn et al., 1999]. In the updated INS data set [Verbruggen et al., 2001] the toxicity data on aldrin and dieldrin were pooled. For sediments no data were present in the INS data sets and therefore information on 1,2-dichloroethane and trichloromethane were taken from the literature [Van Beelen and Van Vlaardingen, 1994; Van Beelen et al., 1994; Van Vlaardingen and Van Beelen, 1992; Van Vlaardingen and Van Beelen, 1994]. This is used as an example since no systematic literature search was performed on sediment toxicity data. For 1,2-dichloroethane and trichloromethane the sensitivity distribution of microbial reactions in sediment was compared with the aquatic SSD. For atrazine, pentachlorophenol, chlordane, copper, cadmium, zinc and lead two different comparisons were made: one based on the comparison between soil processes and aquatic toxicity tests, another one based on the comparison between terrestrial and aquatic toxicity tests.

The data in table 1 are sorted according to delta1 shown in the before last column but the soil, sediment and metal tests were kept separate. The differences delta1 range from 1.82 for chlorpyrifos down to - 2.14 for trichloroethene (and even down to - 2.24 for trichloromethane in sediment). The difference between two logarithms can also be expressed as a ratio. This indicates that for chlorpyrifos, the aquatic toxicity tests were $10^{1.82}$ = 66 times more sensitive than the terrestrial toxicity tests, whereas for trichloroethene, the aquatic toxicity tests were $10^{2.14}$ = 138 times less sensitive than the terrestrial toxicity tests. For chlorpyrifos and atrazine the EqP transformed terrestrial toxicity data were higher than the aquatic toxicity data, whereas it was the other way around for 2,4,6-trichlorophenol and trichloroethene. In other words, the application of the EqP-method gave rise to significant differences for 4 of the 11 organic substances. For the metals half of the comparisons show a significant difference delta1 between the EqP transformed terrestrial data and the aquatic data. For copper and cadmium the aquatic toxicity tests were more sensitive whereas for chromium, arsenic and lead the terrestrial toxicity tests were more sensitive.

For 1,2-dichloroethane and trichloromethane sediment toxicity data were available using microbial processes in anaerobic sediment [Van Beelen and Van Vlaardingen, 1994]. The processes involved were the mineralization of acetate [Van Vlaardingen and Van Beelen, 1994], benzoate [Van Beelen and Van Vlaardingen, 1994], 4-chlorophenol [Van Beelen and Van Vlaardingen, 1994], chloroform [Van Beelen et al., 1994] and methanogenesis [Van Vlaardingen and Van Beelen, 1992]. These processes were performed in sediment with 4.6, 4.4, 7.3, 4, and 3.2 % carbon, respectively. These sediment data are only presented as illustration because sediment data were not present in the original nor in the updated INS data sets [De Bruijn et al., 1999; Verbruggen et al., 2001]. These results suggest that the application of the EqP-method can also give a significant (more than hundredfold) underestimation of the sensitivity of microbial processes in sediment, but the data are much too scarce to draw firm conclusions.

In summary, table 1 shows that the application of the EqP-method on aquatic toxicity data can give significant differences with terrestrial toxicity data for approximately half of the compounds. These differences do not indicate a systematic over- or underestimation, but rather an added uncertainty caused by the application of the EqP-method.

3.2 Can the differences be explained by differences in the reported Kp values?

Now that it has been shown that the EqP-method deviates significantly for approximately half of the tested compounds, the question arises whether this might be attributed to the selection of the Kp values. When the average log EC50soil and the average log EC50water are known one can calculate the "optimized" Kp value (Kp') using a logarithmic transformation of equation {1}:

log EC50soil - log EC50water = log Kp' {12}

This log Kp' value will be referred to as the "optimized" log Kp' value for the EqP-method. For this Kp' value the difference between the average EqP transformed terrestrial log EC50 value and the average aquatic log EC50 value is zero. Table 1 shows this optimized log Kp' value in the third column from the right, which can be compared with Koc values from the literature [MacKay et al., 1997a; MacKay et al., 1997b; MacKay et al., 1997c]. These Koc values were converted to Kp values for a standard soil using equation {3}. The lowest values are listed in the column marked "low" whereas the highest values are listed in the column marked "high". The comparison shows that the log Kp' value falls one log unit (a factor 10) outside the range of the experimental log Kp values for chlorpyrifos, trichloroethene and trichloromethane. Therefore the EqP-method is not valid for the data set of these organic compounds. Neither the statistical uncertainty in the aquatic and terrestrial toxicity values nor the statistical uncertainty in the Kp values is sufficient to explain the difference between the EqP transformed terrestrial data and the aquatic data for these organic compounds. The difference might be attributed to the choice of test species. For trichloroethene and trichloromethane sensitive microbial processes were compared with aquatic toxicity tests. For chlorpyrifos insensitive tests with earthworms contributed for 6 of the 7 terrestrial data. The one test with a springtail was more than a factor 100 more sensitive. It might be possible that chlorpyrifos was less bioavailable in the worm tests.

For metals a different comparison is made because the range of Kp values for metals in different soils is very large and cannot easily be standardized [Otte et al., 2001]. The fourth column from the left shows the log Kp values which were used previously for the determination of sediment quality standards [VROM, 1999]. It is clear that these values are often one unit lower than the log Kp values which are currently used [Otte et al., 2001]. For metals delta1 lies within the range of 0.89 for copper and - 1.03 for lead. These differences might be caused by the selection of the Kp values from the literature.

In summary, the differences between the EqP transformed terrestrial toxicity data and the aquatic toxicity data might be explained by differences in the reported Kp values for most of the compounds but not for chlorpyrifos, trichloroethene and trichloromethane. For the latter compounds the differences might be attributed to the selection of test species.

3.3 How large are the differences between the HC5 calculated from aquatic toxicity data and the HC5 calculated from soil or sediment toxicity data?

The EqP-method is often used for setting soil quality standards to calculate a soil HC5 value in mg/kg from a water HC5 value in μg/liter. The HC5 value is dependent on the average and the standard deviation of the SSD and can be calculated using equation {8} or {9}. The difference between the EqP transformed terrestrial or sediment log HC5 value and the aquatic log HC5 value is called delta2. This difference can be calculated using equation {11} and is listed in the last column of table 1. This difference quantifies the additional uncertainty caused by the application of the EqP-method. Delta2 can also be viewed as the logarithm of the ratio between the EqP transformed terrestrial HC5 and the aquatic HC5. When the EqP-method performs perfectly, both HC5 values are equal and therefore delta2 = log 1 = 0. When the EqP-method is performed to estimate the terrestrial HC5 from the aquatic toxicity data using the aquatic SSD values in table 1, the terrestrial HC5 would be overestimated. The overestimation factor is $10^{1.7}$= 50 for trichloroethene, $10^{1.31}$ = 20 for chromium, more than 10 for chlordane, carbofuran, chlorpyrifos, copper, cadmium and cobalt, upto $10^{2.14}$= 138 for atrazine. For the other compounds the under- or overestimation would be less than a factor 10.

The estimation of a sediment HC5 from aquatic toxicity data also seems to be subjected to large uncertainties. For trichloromethane the sediment HC5 would have been underestimated with a factor $10^{2.63}$ = 427. This large ratio might be attributed to the large differences in sensitivity for trichloromethane between the anaerobic processes in sediment and aquatic toxicity tests [Van Beelen and Van Vlaardingen, 1994].

In summary: The use of the EqP-method to estimate terrestrial HC5 values from aquatic HC5 values can lead to both over- and underestimations which can occasionally be one or even two orders of magnitude.

3.4 The quantification of the extra uncertainty caused by the application of the EqP-method in soil

The preceding paragraphs have shown that the application of the EqP-method did not lead to a systematic over- or underestimation of the terrestrial HC5 for the selected organic compounds and metals. For a specific compound however a serious over- or underestimation of the terrestrial HC5 by the application of the EqP-method can occur. Provided that the terrestrial data are of the same quality as the aquatic data, the terrestrial HC5, which is derived using the EqP-method is less reliable than a terrestrial HC5 which is derived from soil toxicity tests. This extra uncertainty caused by the use of the EqP-method can be quantified using the difference between the terrestrial log HC5 and the aquatic log HC5 shown as delta2 in the last column of table 1. For organic compounds delta2 ranged between 2.14 and -1.7 . When the sediment data are left out, 13 delta2 values remain, which can be described by a distribution with an average of 0.36 and a standard deviation of 1.02. The lower dotted line in figure 1 shows this distribution. The delta2 values for organic compounds are shown as squares and are distributed evenly on the vertical scale starting with the lowest value to get a cumulative distribution [Aldenberg and Jaworska, 2000]. On average, the EqP-method performs well for the organic compounds in soil since the average of the distribution (0.36) is close to 0. When one is interested in a specific HC5 for a specific compound the broadness of the distribution can pose a problem because the difference caused by the application of the EqP-method can be two orders of magnitude (see figure 1). The lower 5% confidence interval of this distribution is important because it can be used to quantify the extra uncertainty caused by the EqP-method. This confidence interval can be calculated from the average (0.36), the standard deviation (1.02) and the number of data (13) from this distribution. The statistical method of Aldenberg and Jaworska [2000] (which gives an extrapolation factor of 1.686997) yields 0.36 - 1.686997*1.02 = -1.37. This indicates that the estimation of the soil HC5 from the aquatic HC5 using the EqP-method is less than a factor $10^{1.37}$ = 23 too large in 95% of the cases. The upper 5% confidence interval can be calculated accordingly giving: 0.36 + 1.686997*1.02 = 2.08. This indicates that the estimation of the soil HC5 from the aquatic HC5 using the EqP-method is less than a factor 120 too small in 95% of the cases.

The application of the EqP-method for sediments can give rise to even larger uncertainties. For organic compounds, the ratio between the $HC5^{EC50}$water and the $HC5^{EC50}$sediment can be as large as $10^{-2.63}$ = 427 (- 2.63 is the left most point in figure 1 for trichloromethane in sediment). But more data are needed to estimate a reliable safety factor.

For metals, the log transformed ratio between the aquatic HC5 and the terrestrial HC5 ranged between 1.75 and - 1.31 (see table 1). A number of 12 ratios are used, which can be described by a distribution with an average of 0.14 and a standard deviation of 0.899. The upper dotted line in figure 1 shows this distribution, while the individual ratios are marked as triangles. Again a 95% confidence interval can be calculated using the method of Aldenberg and Jaworska (2000) for this distribution with a slightly different extrapolation factor of 1.6910 for 12 data. This gives 0.14- 1.6910*0.899 = - 1.38. This indicates that the estimation of the soil HC5 from the aquatic HC5 using the EqP-method is less than a factor 24 too large in 95% of the comparisons with metals. The upper 5% confidence interval can be calculated accordingly giving: 0.14 + 1.6910*0.899 = 1.66. This indicates that the estimation of the soil HC5 from the aquatic HC5 using the EqP-method is less than a factor 46 too small in 95% of the cases.

When all the data for the log transformed ratio between the aquatic HC5 and the terrestrial or sediment HC5 are joined together. One gets a distribution with 27 delta2 values with an average of 0.09 and a standard deviation of 1.107. For 27 data the Aldenberg and Jaworska method (2000) gives an extrapolation factor of 1.663978. This would yield a factor of 0.09- 1.663978*1.107 = - 1.7568. A log transformation would give an underestimation factor of 57. The corresponding overestimation factor can be calculated using 0.09 + 1.663978*1.107 = 1.932. Which means that the overestimation factor is 86. This factor is lower than the overestimation factor of 120 for the organic compounds but higher than the overestimation factor of 46 for the metals. This indicates that the use of the EqP-method to derive soil HC5 values from aquatic toxicity data might lead to HC5 values which are two orders of magnitude too low and are therefore overprotective.
The underestimation factors, on the other hand, range from 57 for the total data set to 23 for organic compounds or 24 for metals. The value of 57 is caused by the comparison between sediment processes and aquatic organisms which are taxonomically unrelated. Therefore only the values of 23 and 24 are selected. These values are only an order of magnitude estimation and depend on the selected toxicity data and Kp values. Rounding off to the nearest factor of ten gives 20. This indicates that the use of the EqP-method to derive soil HC5 values from aquatic toxicity data can lead to HC5 values which are for 5% of the compounds more than a factor of 20 too high and are therefore underprotective.

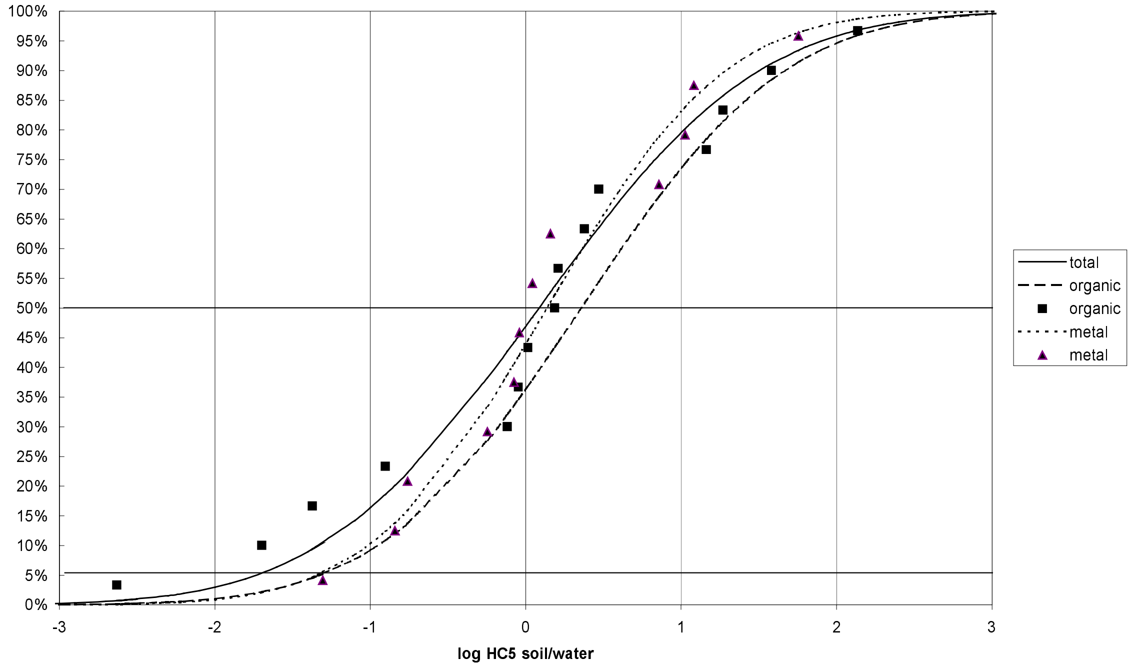

Figure 1 The difference between model and observations.

The difference between model and observations is expressed as the cumulative distribution of the log transformed ratios between the EqP transformed terrestrial HC5 and the aquatic HC5, (delta2) for each of the compounds listed in table 1. The compounds on the left hand side of the figure (the negative values) would be underprotected when the EqP-method was used to derive a terrestrial HC5 from aquatic toxicity data. For the 4 compounds left of - 1 the terrestrial HC5 was more than a factor 10 smaller than the terrestrial HC5 derived from aquatic data. For the 7 compounds to the right of 1 it was the other way around.

3.5 How can the observed differences, caused by the application of the EqP-method, be explained and do they match with earlier findings?

In the above paragraphs it was shown that the EqP-method deviated significantly for almost half of the tested compounds from the updated INS data set. The following factors contributed to this deviation:

1. Differences between species sensitivity distributions in water and either sediment or soil.
2. Differences in exposure conditions during the toxicity tests in water, soils and sediments.
3. Differences in sensitivity of test species within the updated INS data set.
4. Selection of the Kp value from the literature.

Both the Technical Commission Soil Protection [TCB, 1994] and the Dutch Health Council [Gezondheidsraad, 1995] have stated that the EqP-method is not recommended for compounds like metals and pesticides. The data analysis in this report confirms that toxicity tests with soil and sediment are necessary for a reliable and accurate determination of soil and sediment MPC values. This supports the standing practice in the Netherlands, where the EqP-method is only used when insufficient soil or sediment toxicity data are available. At this stage, the question about how many data should be regarded as insufficient can now be answered in more detail. One must bear in mind that the recommendations in the next paragraph are only suited for very crude estimations. The use of a limited amount of terrestrial toxicity data can lead to an uncertainty in the estimation of the terrestrial HC5, which is much more than the factor 20 attributed to the use of the EqP-method.

3.6 How many terrestrial toxicity data are required to estimate an HC5 value that is more accurate than the one derived from aquatic toxicity data using the EqP-method?

In appendix 1, it is shown that the large uncertainty caused by the use of a limited amount of terrestrial toxicity data can be quantified.This uncertainty factor can be compared with the uncertainty factor 20 caused by the use of the EqP-method (provided that sufficient aquatic toxicity data and sorption data are available). The first 4 recommendations show the outcome of this comparison.

4. Recommendations

1 When less than 4 terrestrial toxicity data are available, the use of the EqP-method can be advocated because the uncertainty in the estimation of the HC5 is much larger than a factor 20.

2 When 4 terrestrial toxicity data are available for a narcotic toxicant, the use of the terrestrial data is preferred. When the terrestrial data have a large standard deviation and there is sufficient information about the sorption behavior and the aquatic toxicity, the use of the EqP-method can also be advocated.

3 When more than 4 terrestrial toxicity data are available it is generally better to use these data instead of using the EqP-method to derive a HC5 value from aquatic data.

4 In special cases, for a compound which has a large standard deviation of its aquatic Species Sensitivity Distribution and which has an accurate Kp value and a lot of reliable aquatic toxicity data covering a large taxonomic diversity, it might be better to use the EqP-method even when 5, 6 or 7 terrestrial toxicity data are available. The uncertainty in the HC5 from 7 data with a standard deviation of 1.5 is a factor 317 (shown in *table 2*), which is much larger than a factor 20.

5 The HC5 values which are based on less than five toxicity data or which are derived using the (modified) EqP-method should be regarded as preliminary HC5 values. These preliminary HC5 values can be used in comparison with environmental concentrations in order to decide whether more research is needed for the risk evaluation of a specific pollutant.

6 More sediment toxicity data should be acquired to determine reliable sediment MPCs.

5. Conclusions

The use of the EqP-method to derive a terrestrial HC5 from sorption data and aquatic toxicity data gave an approximately equal chance of underestimation or overestimation. The EqP-method deviated significantly for approximately half of the tested compounds from the updated INS data set. In 5% of the tested compounds, the overestimation of the terrestrial HC5 derived from aquatic data, was more than a factor 20.

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References

Aldenberg T., Jaworska J.S. 2000. Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. Ecotoxicol. Environ. Saf. 46: 1-18.

Armitage P., Berry G. 1994. Statistical methods in medical research. Cambridge, United Kingdom: Blackwell Science.

Bockting G.J.M., Van De Plassche E.J., Struijs J., Canton J.H. 1993. Soil-water partition coefficients for organic compounds. Bilthoven, the Netherlands: National Institute of Public Health and Environmental Protection (RIVM). Report No. 679101013.

Crommentuijn T., Polder M., Sijm D., De Bruijn J., Van De Plassche E. 2000a. Evaluation of the Dutch environmental risk limits for metals by application of the added risk approach. Environ. Toxicol. Chem. 19: 1692-1701.

Crommentuijn T., Sijm D., De Bruijn J., Van Den Hoop M., Van Leeuwen K., Van De Plassche E. 2000b. Maximum permissible and negligible concentrations for metals and metalloids in the Netherlands taking into account background concentrations. Journal of Environmental Management. 60: 121-143.

Crommentuijn T., Sijm D., De Bruijn J., Van Leeuwen K., Van De Plassche E. 2000c. Maximum permissible and negligible concentrations for some organic substances and pesticides. Journal of Environmental Management. 58: 297-312.

De Bruijn J., Crommentuijn T., Van Leeuwen K., Van De Plassche E., Sijm D., Van Der Weiden M. 1999. Environmental Risk Limits in The Netherlands. Bilthoven, the Netherlands: National Institute of Public Health and Environmental Protection (RIVM). Report No. 601640001.

Di Toro D.M., Zarba C.S., Hansen D.J., Berry W.J., Swartz R.C., Cowan C.E., Pavlou S.P., Allen H.E., Thoma N.A., Paquin P.R. 1991. Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. Environ. Toxicol. Chem. 10: 1541-1583.

EC. 1996. Technical Guidance Documents in support of Directive 93/67/EEC on risk assessment of new notified substances and Regulation (EC) No. 488/9 on risk assessment of new notified substances (Parts I, II, III and IV). Report No. EC catalogue numbers CR-48-96-001, 002, 003, 004-EN-C. 2 rue Mercier, L-2965 Luxembourg.: Office for Official Publications of the European Community.

Gezondheidsraad. 1995. Het project integrale normstelling stoffen. Report No. 1995/07. Den Haag

Hoekstra J.A, Van Ewijk P.H. 1993. Alternatives for the no-observed-effect level. Environ. Toxicol. Chem. 12: 187-195.

Kalf D.F., Mensink B.J.W.G., Montforts M.H.M.M. 1999. Protocol for the derivation of Harmonised Maximum Permissible Concentrations (MTRs). Bilthoven, the Netherlands: National Institute of Public Health and Environmental Protection (RIVM). Report No. 601506001.

Lijzen J.P.A., Baars A.J., Otte P.F., Rikken M., Swartjes F.A., Verbruggen E.M.J., Van Wezel A.P. 2001. Technical evaluation of the Intervention Values for Soil/sediment and Groundwater. Human and ecotoxicological risk assessment and derivation of risk limits for soil, aquatic sediment and groundwater. Bilthoven, the Netherlands: National Institute of Public Health and Environmental Protection (RIVM). Report No. 711701023.

MacKay D., Shiu, Ma. 1997a. Monoaromatic Hydrocarbons, Chlorobenzenes and PCBs. Illustrated handbook of physical-chemical properties and environmental fate for organic chemicalsVol. 1). Boca Raton, Florida: Lewis Publishers.

MacKay D., Shiu, Ma. 1997b. Pesticide chemicals. Illustrated handbook of physical-chemical properties and environmental fate for organic chemicalsVol. 5). Boca Raton, Florida: Lewis Publishers.

MacKay D., Shiu, Ma. 1997c. Volatile Organic Chemicals. Illustrated handbook of physical-chemical properties and environmental fate for organic chemicalsVol. 3). Boca Raton, Florida: Lewis Publishers.

Otte P.F., Lijzen J.P.A., Otte J.G., Swartjes F.A., Versluijs C.W. 2001. Evaluation and revision of the CSOIL parameter set. Proposed parameter set for human exposure modelling and deriving Intervention Values for the first series of compounds. Bilthoven, the Netherlands: National Institute of Public Health and Environmental Protection (RIVM). Report No. 711701021.

TCB. 1994. Advies project Integrale Normstelling Stoffen deel b. Report No. Ao9. Leidschendam:

Traas T.P. 2001. Guidance document on deriving environmental risk limits. Bilthoven, the Netherlands: National Institute of Public Health and Environmental Protection (RIVM). Report No. 601501012.

Vaal M.A., Van Leeuwen C.J., Hoekstra J.A., Hermens J.L.M. 2000. Variation in sensitivity of aquatic species to toxicants: practical consequences for effect assessment of chemical substances. Environ. Manag. 25: 415-423.

Van Beelen P., Van Vlaardingen P.L.A. 1994. Toxic effects of pollutants on the mineralization of 4-chlorophenol and benzoate in methanogenic river sediment. Environ. Toxicol. Chem. 13: 1051-1060.

Van Beelen P., Van Vlaardingen P.L.A., Fleuren-Kemilä A.K. 1994. Toxic effects of pollutants on the mineralization of chloroform in river sediments. Ecotoxicol. Environ. Saf. 27: 158-167.

Van Straalen N.M., Denneman C.A.J. 1989. Ecotoxicological evaluation of soil quality criteria. Ecotoxicol. Environ. Saf. 18: 241-251.

Van Vlaardingen P.L.A., Van Beelen P. 1992. Toxic effects of pollutants on methane production in sediments of the river Rhine. Bull. Environ. Contam. Toxicol. 49: 780-786.

Van Vlaardingen P.L.A., Van Beelen P. 1994. Toxic effects of pollutants on the mineralization of acetate in methanogenic river sediment. Bull. Environ. Contam. Toxicol. 52: 46-53.

Verbruggen E.M.J., Posthumus R., Van Wezel A.P. 2001. Ecotoxicological Serious Risk Concentrations for soil, sediment and (ground)water: updated proposals for first series of compounds. Bilthoven, the Netherlands: National Institute of Public Health and Environmental Protection (RIVM). Report No. 711701020.

VROM. 1999. Integrale normstelling stoffen: milieukwaliteitsnormen bodem, water, lucht ; geactualiseerde versie INS-notitie 1997. Report, Den Haag: Ministerie van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer.

Appendix 1 Quantification of uncertainty

The quantification of the uncertainty caused by the application the statistical extrapolation method on a limited number of toxicity data

The ratio of the median HC5 and the lower 5% confidence level of the HC5 can quantify the uncertainty in the HC5 value (UF). The median HC5 can be calculated according to equation {8} using the median extrapolation constant (mc), while the lower HC5 can be calculated in the same way using the lower extrapolation constant (lc).

log UF = Log (HC5median/HC5lower) = log HC5median - log HC5lower {13}

Using equation {8} yields:

logUF=average(logNOEC)-mc*SD(logNOEC)-average(logNOEC)+lc*SD(logNOEC)

logUF=(lc-mc)*SD(logNOEC) {14}

The uncertainty factor UF is dependent on the standard deviation of the toxicity data and on the extrapolation constants, which are dependent on the number of species tested. Table 2 shows that UF decreases strongly at increasing number of test species and that the UF increases for compounds with a higher standard deviation. Narcotic compounds normally have a standard deviation below 0.3 [Vaal et al., 1997] whereas table 1 shows that the standard deviation of most pesticides and metals are in the range of 0.5 to 1. When UF is above 1000 we assume that the corresponding HC5 value is too uncertain to be of much use and it is therefore better to use the EqP-method instead of an insufficient number of terrestrial toxicity data. On the other hand, when UF is below 20 it can be assumed that the uncertainty caused by the low number of test species is smaller than the uncertainty caused by the application of the EqP-method. Table 2 shows that for n = 2 the UF is above 1000 for all the tabulated standard deviations. In other words, when less than 3 terrestrial toxicity data are available it is more accurate to use the EqP-method than to rely on only a very limited amount of terrestrial toxicity data.

The right column in table 2 shows the uncertainty factor UF for compounds with a very specific mode of action like certain antibiotics, insecticides or herbicides that have a SSD with a large standard deviation. For these compounds it is of the utmost importance that a large number of different species are tested since there is a risk that one might miss the most sensitive taxonomic group. Even when 8 terrestrial species are tested the uncertainty factor UF is 160 which indicates that the uncertainty due to the limited number of terrestrial species is still much larger than the factor 20 which is caused by the application of the EqP-method. In practice it is often known which taxonomic group is more at risk and therefore the uncertainty due to the limited number of terrestrial species can be smaller because the species are not selected random.

Table 2. The relation between the number of test species and the standard deviation of the sensitivity distribution on the ratio between the median and the lower estimate of the HC5

No. species	SD=0.3	SD=0.5	SD=0.7	SD=1	SD=1.5
2	2.E+07	9.E+11	6.E+16	8.E+23	8.E+35
3	52	722	1.E+04	5.E+05	4.E+08
4	*10*	45	209	2.E+03	9.E+04
5	*5*	*16*	50	265	4.E+03
6	*4*	*10*	*23*	91	863
7	*3*	*7*	*15*	47	317
8	*3*	*5*	*11*	29	160
9	*2*	*5*	*8*	*21*	96
10	*2*	*4*	*7*	*16*	65
11	*2*	*4*	*6*	*13*	48
12	*2*	*3*	*5*	*11*	37
13	*2*	*3*	*5*	*10*	30
14	*2*	*3*	*4*	*9*	25
15	*2*	*3*	*4*	*8*	*21*

Appendix 2 Mailing list

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Table 1. Comparison between the Species Sensitivity Distributions from log EC50 or log NOEC values from aquatic and terrestrial toxicity tests using the EqP-method

	Soil					Water					Partitioning coefficients				Comparisons	
Substance	**Parameter**	**Avr**	**SD**	**N**	**HC5**	**Parameter**	**avrg**	**SD**	**N**	**HC5**	**log Kp**	**low**	**high**	**log Kp'**	**delta1**	**delta2**
Chlorpyrifos	log EC50	2.25	1.25	7	1.2	log EC50	0.86	1.17	42	0.08	2.58	0.37	3.13	4.40	**1.82**	1.58
Atrazine	log NOEC	1.55	0.55	5	4	log NOEC	1.88	0.85	23	2.9	0.97	-0.54	2.89	2.67	**1.70**	**2.14**
Carbofuran	log EC50	0.62	0.95	7	0.09	log EC50	2.00	0.95	14	2.5	0.41	-0.24	1.46	1.62	*1.21*	1.16
Pentachlorophenol	log NOEC(P)	1.86	1.08	23	1.1	log NOEC	1.99	0.77	42	5	1.97	2.25	4.47	2.87	**0.90**	0.38
Chlordane	log NOEC(P)	0.88	0.62	6	0.6	log NOEC	-0.23	0.90	8	0.016	3.30	3.06	4.33	4.11	0.81	*1.27*
Atrazine	log NOEC(P)	0.49	0.86	4	0.08	log NOEC	1.88	0.85	23	3	0.97	-0.54	2.89	1.61	0.64	0.47
Pentachlorophenol	log NOEC	1.19	0.85	4	0.4	log NOEC	1.99	0.77	42	5	1.97	2.25	4.47	2.21	0.24	-0.05
Chlordane	log EC50	1.19	0.41	5	3	log EC50	1.13	0.71	30	0.9	3.30	3.06	4.51	3.06	-0.24	0.21
Aldrin dieldrin	log EC50	0.36	0.46	6	0.4	log EC50	0.87	0.66	70	0.6	2.76	1.37	3.45	2.49	-0.26	0.01
1,2,4-Trichlorobenzene	log EC50	2.29	0.11	5	122	log EC50	3.54	0.41	11	707	2.05	2.31	3.16	1.75	*-0.30*	0.19
Heptachlor	log EC50	0.56	0.90	6	0.10	log EC50	1.19	0.88	37	0.5	3.15	2.57	3.14	2.36	-0.79	*-0.90*
2,4,6-Trichlorophenol	log EC50	1.91	0.10	5	54	log EC50	3.87	0.74	19	425	2.22	0.80	2.10	1.04	**-1.18**	-0.12
Trichloroethene	log NOEC(P)	0.39	0.45	5	0.4	log NOEC	4.70	0.71	6	2903	0.83	1.04	2.33	-1.31	**-2.14**	*-1.70*
1,2-Dichloroethane	log EC50(S)	2.45	1.38	5	1.0	log EC50	5.18	0.64	13	12729	0.25	-0.15	0.27	0.27	0.02	*-1.37*
Trichloromethane	log EC50(S)	0.18	0.64	4	0.10	log EC50	4.99	0.46	12	16302	0.42	0.20	1.55	-1.82	**-2.24**	**-2.63**
Copper	log NOEC	2.48	0.65	12	25	log NOEC	1.26	0.74	87	1.1	3.33	2.99		4.22	**0.89**	**1.03**
Cadmium	log NOEC(P)	2.06	0.63	70	10	log NOEC	1.19	1.01	87	0.3	3.41	2.30		3.87	**0.46**	**1.08**
Cobalt	log NOEC(P)	2.22	0.55	26	21	log NOEC	2.91	1.41	8	3	2.08	1.60		2.32	0.24	**1.75**
Zinc	log NOEC	2.59	0.26	7	136	log NOEC	1.95	0.66	49	7	3.41	2.20		3.64	0.22	**0.86**
Copper	log NOEC(P)	1.78	0.76	59	3	log NOEC	1.26	0.74	87	1.1	3.33	2.99		3.52	0.19	0.16
Zinc	log NOEC(P)	2.32	0.67	27	16	log NOEC	1.95	0.66	49	7	3.41	2.20		3.37	-0.05	-0.08
Mercury	log NOEC(P)	1.55	0.76	18	2	log NOEC	0.80	0.86	38	0.23	3.88	2.23		3.75	-0.12	0.04
Cadmium	log NOEC	1.08	0.70	13	0.8	log NOEC	1.19	1.01	87	0.3	3.41	2.30		2.89	-0.52	-0.04
Chromium III	log NOEC(P)	2.13	0.72	37	9	log NOEC	2.35	0.46	7	36	3.68	2.04		2.78	**-0.90**	**-1.31**
Arsenic	log NOEC(P)	2.21	0.49	20	25	log NOEC	2.95	0.93	17	24	3.26	2.28		2.26	**-0.99**	*-0.25*
Lead	log NOEC(P)	2.72	0.59	39	55	log NOEC	2.17	0.69	42	11	4.56	3.28		3.55	**-1.00**	**-0.84**
Lead	log NOEC	2.69	0.52	13	66	log NOEC	2.17	0.69	42	11	4.56	3.28		3.53	**-1.03**	**-0.76**
Organic substances															0.19	0.36
Metals															-0.22	0.14
Total															-0.09	0.09

The difference between the logarithmically transformed terrestrial toxicity data (expressed in mg/kg) and the logarithmically transformed aquatic toxicity data (in µg/liter) is called delta1 and is calculated according to equation {6}. The difference between the aquatic log HC5 and the terrestrial log HC5 is called delta2 and is calculated using equation {11}. Significant differences below 1% probability are printed **bold** and the significant differences below 5% are printed in *italics.*