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Summary

Environmental quality standards (EQSs) are frequently used in environmental regulation. They are derived according to standardized approaches, e.g. by applying safety factors to ecotoxicity values for the most sensitive species, or by a method based on the distribution of sensitivities across a set of species (the Species Sensitivity Distribution method, SSD). The criteria are used to prevent and limit environmental contamination, but also to judge existing contamination. The latter introduces a conflict: the lower the EQS, the better the environment is protected against novel contamination, but the larger the environmental volume or surface that is apparently contaminated. Unnecessarily low EQSs can therefore lead to a waste of money on remediation that does not lead to a higher environmental quality.

This report focuses on the derivation of EQSs, and specifically considers the impact of additional ecotoxicity data on both the level of the EQSs themselves, as well as the consequences for environmental management of that. Novel ecotoxicity data are obtained by four extrapolation methods. The results suggest that the EQSs derived by the SSD method often increase as a result of adding an extra NOEC (No-observed effect concentration). Given that those criteria would be accepted within existing regulations, the consequences for environmental management are illustrated using a case study. The case study concerns the deposition of contaminated freshwater sediment in the Netherlands. The example illustrates the friction between urgent water quantity management needs and potential long-term soil contamination. It shows that slight increases of EQSs would imply a large reduction of risk management costs, without causing soil contamination beyond a level accepted within the context of the existing Guidance Documents.

Content

1 Introduction

Ecological risk assessment is defined as a process that evaluates the likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors (U.S. Environmental Protection Agency, 1992). Risk assessors often find themselves in data-sparse situations, which leads to uncertain estimations. A general regulatory principle in environmental management is that the use of additional information for risk assessments will reduce uncertainty, resulting in assessments that are more accurate and the application of less stringent safety margins. For example, in the derivation of environmental quality standards (EQSs), large safety factors are applied if little data is available and vice versa. As conservative EQSs lead to a waste of money due to unnecessary measures, and too lenient standards can lead to unexpected adverse effects and high remediation costs, it is important that EQSs are well underpinned. In the present study, we investigated the influence of the sample size of toxicity data on EQSs derived by using Species Sensitivity Distributions (SSDs).

As described by Forbes and Calow (2002) uncertainty of SSDs is introduced by assumptions behind their theory and application. Various studies on the importance of model choice, the quality and quantity of toxicity data, the selection of species and the relevance of SSDs for deriving EQSs have been performed over the last years (Maltby et al., 2005; Newman et al., 2000; Posthuma et al., 2002; Wheeler et al., 2002). Recent research on SSDs has mainly focused on integration of interactions between species within an ecosystem into SSDs (De Laender et al., 2008a; De Laender et al., 2008b) and on alternatives to animal testing in an attempt to increase the sample size (Dyer et al., 2008). The present study aims to quantify the impact of gathering additional toxicity data on EQSs and their uncertainty.

A case study on polluted sediment in the Netherlands is presented to illustrate that additional data can result in less stringent EQSs due to uncertainty reduction, without causing adverse environmental impacts. Sediment contamination currently constitutes a problem in risk management in the Netherlands because of high costs. Regular removal of sediments is an essential part of water quantity management. Each year 20 million m^3 of fresh water sediment is dredged in the Netherlands (Advies en Kenniscentrum Waterbodems, 2001). Depending on the level of contamination, sediment can be dispersed on land, discharged in water, stored in depots or remediated. If classification rules are too strict, this means that the amount of sediment dispersed on land or discharged in water is suboptimal and costs will be higher than necessary, while rules that are too lenient may cause environmental damage. The aims of the study are to quantify the uncertainty of EQSs derived by the SSD method, predict the impact of adding an extra no-observed effect concentration (NOEC) to the available dataset and compare the costs of the extra NOEC with the potential financial benefits of the new EQS. This study is not meant to be an extensive cost-benefit analysis as performed by Brouwer and De Blois (2008) or Van Wezel et al. (2008), but shows that the effort of striving for an optimal derivation of the EQS is likely to be financially rewarded.

2 Materials and Methods

2.1 Case study

A case study on polluted sediment in the Netherlands was chosen to illustrate the consequences of adding extra toxicity data. In the Netherlands, sediment is divided into five classes (Van de Guchte et al., 2000); class 0 and class 4 represent clean sediment and highly contaminated sediment, respectively (see Figure 2.1). Sediment belonging to class 0, 1 or 2 is allowed to be dispersed, whereas sediment from class 3 or 4 has to be stored or remediated. The relation between sediment classes and EQSs is complex. Sediment policy and regulations are subjects to change, which makes it rather difficult to give a clear and realistic representation of the background of the sediment classes. In the present study, the following boundaries are used which are in line with the Dutch policy for polluted sediments:

- class 0 – class 1: Negligible Concentration (NC)
- class 1 – class 2: Maximum Permissible Concentration (MPC)
- class 2 – class 3: Limit between dispersible and non-dispersible sediment ($EQS_{d\text{-}nd}$)
- class 3 – class 4: Intervention Value (IV)

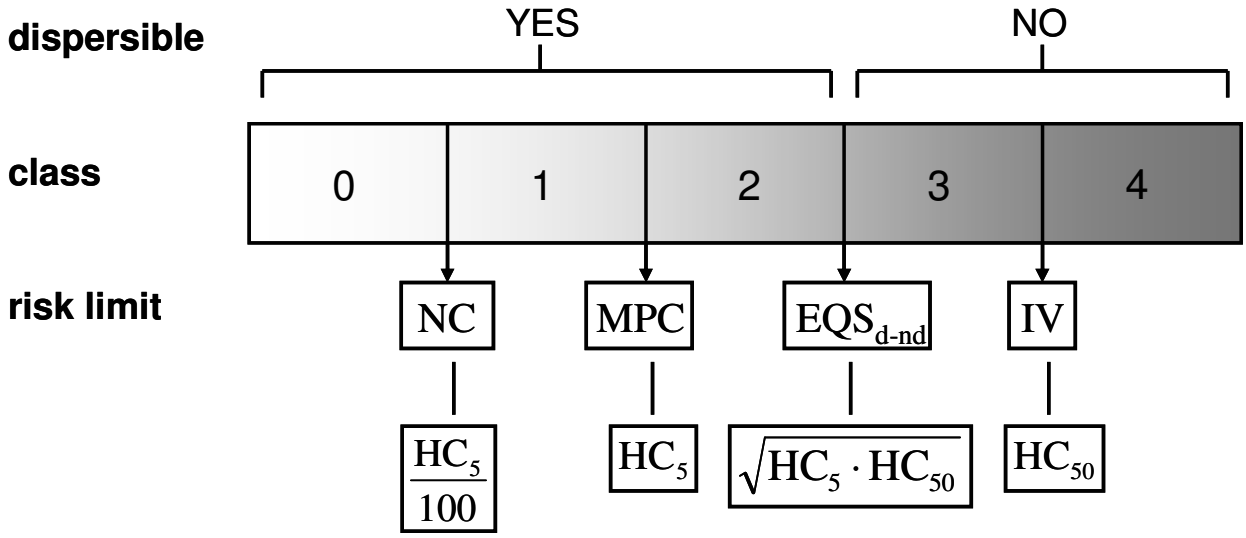


Figure 2.1: Classification system of sediment in the Netherlands. Class 0 is clean sediment, whereas class 4 is the most polluted sediment. Sediment from class 0, 1 or 2 is allowed to be dispersed, whereas sediment from class 3 and 4 has to be stored or remediated.

These EQSs can be derived with the SSD method or the assessment factor method. In the past, Dutch EQSs have not always been derived in a consistent way. Sometimes calculated EQS values had been adapted due to policy decisions. In our study, we applied the SSD method and the EQSs are defined as follows. The MPC is defined as the concentration at which 95% of the species are protected (HC_5: hazardous concentration for 5% of the species). The NC is calculated by dividing the MPC by a factor of 100. The IV is defined as the concentration at which 50% of the species are protected (HC_{50}). Based on the report of Wezenbeek (2007) it is assumed that the $EQS_{d\text{-}nd}$ lies between the MPC and the IV. It is calculated as the geometric mean of these two values. When the HC_5 or HC_{50} is represented by a probability distribution (reflecting uncertainty), the median value of this distribution is used as the EQS.

In addition to analyzing the change of the HC_5, HC_{50} and $EQS_{d\text{-}nd}$ caused by adding an extra NOEC, the change in amount of dispersible and non-dispersible sediment and the resulting potential financial benefits or drawbacks were investigated. Concentration data for a large number of sediment dredging loads were collected from an extensive database of the Water Service of the Directorate-General for Public Works and Water Management (Oste et al., 2008). These water quality data originate from 1992-2005. To give an example on the change in remediation costs, we estimated the volume of the sediment loads by using the median volume of sediments loads from the Prospect database from the Water Service and AKWA (Advies en Kenniscentrum Waterbodems, 2001), which was 2625 m^3. The change in non-dispersible volume was determined by comparing the measured chemical concentration of the sediment loads with the old $EQS_{d\text{-}nd}$ (original set of NOECs) and the new $EQS_{d\text{-}nd}$ (expanded set of NOECs). These comparisons were done for each chemical separately. In the present study we want to show the change of sediment volumes when changing one EQS by adding one NOEC, therefore, if more than one chemical exceeded its $EQS_{d\text{-}nd}$, the sediment load was not included in the calculations. The database included concentrations of 13100 sediment loads. 427 sediment loads had a concentration of one of the priority chemicals described in paragraph 2.4 exceeding the $EQS_{d\text{-}nd}$. In 92 sediment loads the concentration of more than one chemical exceeded the $EQS_{d\text{-}nd}$. The difference in costs for dispersible and non-dispersible sediment is estimated to be €30/m^3 (Advies en Kenniscentrum Waterbodems, 2001).

2.2 Risk limits

The HC_5 and HC_{50} are derived from SSD calculations and represent the concentrations at which 95% and 50% of the species of an ecosystem are protected, respectively. SSDs were derived for several chemicals with different numbers of NOECs available. As recommended by the TGD, we used the method described in Aldenberg and Jaworska (2000), which assumes a normal distribution for toxicity data. The log(HC) for *p*% of the species population is

$$\log(HC_p) = \bar{x} - k_s \cdot s \qquad (1)$$

where $\bar{x}$ and s are the mean and the sample standard deviation of the set of log-transformed toxicity data (NOECs) and k_s is the extrapolation factor which depends on the sample size and the level of confidence of the HC_p chosen (see Aldenberg and Jaworska, 2000 for details).

Since ecotoxicological data on sediment-dwelling species are scarce, risk limits for sediment are generally derived from aquatic ecotoxicity data for freshwater species using the equilibrium partitioning method (European Chemicals Bureau, 2003b). The partitioning of a pollutant between water and a solid phase like sediment, soil or suspended solids can be

described by a partition coefficient (K_p) which is defined as the concentration ratio between the solid and the aqueous phase at equilibrium

$$K_p = C_{solid} / C_{water} \quad (2)$$

where C_{solid} and C_{water} are chemical concentrations in the solid phase and water, respectively. In present study the equilibrium partitioning method was used to derive the HC_5 and HC_{50} for all chemicals in sediments. We did not include uncertainty in K_p-values in this study.

In the results section the change in risk limits (HC_5, HC_{50} and $EQS_{d\text{-}nd}$) and the volume change after adding an extra NOEC are presented. The results of the change of the uncertainty range are given in Appendix A.

2.3 Estimation of aquatic NOECs

In order to estimate the impact of an additional toxicity value on an EQS, new NOECs had to be generated. In the present study, we used four methods to predict new NOECs based on available toxicity values. The newly predicted values were included in the existing dataset to derive a new SSD for each chemical. This enabled a comparison of the old and new EQSs. An overview of the methods is given in Figure 2.2. It is not the purpose to give a detailed description of these methods, but to give a brief overview. For further information we refer to the literature references.

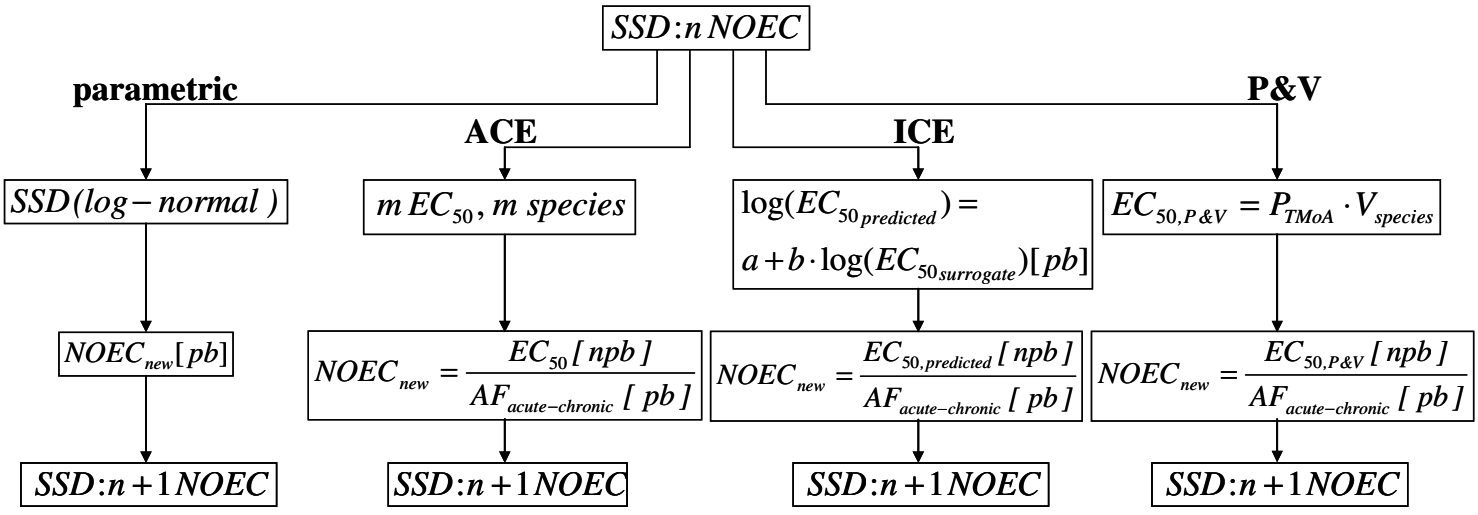


Figure 2.2: Overview of methods used to predict additional NOECs: parametric bootstrapping (parametric), acute to chronic extrapolation (ACE), interspecies correlation estimation (ICE) and potency and vulnerability (P&V). A Monte Carlo simulation was performed making use of parametric and non-parametric bootstrapping (pb and npb). (SSD = species sensitivity distribution, NOEC = no-observed effect concentration; EC50 = effect concentration of 50%; n = number of NOECs; m = number of EC50s; $AF_{acute\text{-}chronic}$ = acute to chronic assessment factor;

PTMoA = potency of certain Toxic Mode of Action; Vspecies = vulnerability of a certain species)

Parametric bootstrapping

Parametric bootstrapping was used in order to estimate new toxicity data based on the distribution of already available toxicity data. For each chemical, a lognormal distribution was fitted to the dataset (NOECs) and a random number was drawn from this distribution. This number functioned as a new NOEC. This NOEC was added to the original dataset and a new SSD was derived. This step was repeated 10.000 times, using Crystal Ball ® 7.1.2 (Decisioneering, 2005). This method is based on the assumption that the toxicity of a certain chemical for a new species will fit into the SSD of the set of known species.

Acute to chronic extrapolation (ACE)

For most species and substances, more data are available on acute toxicity than on chronic toxicity. Therefore, extrapolation of acute to chronic data can be a useful tool to estimate chronic toxicity values for taxonomic groups with unknown chronic toxicity. Much literature is available for the extrapolation of acute to chronic toxicity (Ahlers et al., 2006; Duboudin et al., 2004; Lange et al., 1998; Roelofs et al., 2003). In the present study we chose the method of Roelofs et al. (2003) because it is based on a wide range of aquatic species. Roelofs et al. derived assessment factors ($AF_{acute\text{-}chronic}$) for aquatic species from an extensive ecotoxicological database (De Zwart, 2001) for two different groups of species: microorganisms (Algae, Cyanobacteria, Protozoa and Rotifera) with a median of 4.8 and a 95th percentile of 40.5, and other organisms (Crustacea, bonefish, Amphibia, Annelida, Insecta, Mollusca and Nematoda) with a median of 12.9 and a 95th percentile of 267.6.

Using the $AF_{acute\text{-}chronic}$ of Roelofs et al., chronic data can be calculated as

$$NOEC_{x,s} = \frac{L(E)C_{50\,x,s}}{AF_{acute-chronic}} \tag{3}$$

A NOEC was derived for each chemical and species available, using one of the two acute-chronic extrapolation factors calculated by Roelofs et al. (2003). Only EC_{50}s for species belonging to one of the abovementioned taxonomic groups were used to estimate NOECs. This method, as well as the following two estimation methods, assumed that any aquatic species for which an EC_{50} was available could be the next to be tested. The only restriction was that the new test species should belong to a different taxonomic group than the original set of NOECs. For each chemical, 10,000 new NOEC values were generated by making use of non-parametric bootstrapping for the given L(E)C50s and parametric bootstrapping of the $AF_{acute\text{-}chronic}$. These NOECs were used as input data for newly derived SSDs.

Interspecies correlation estimation models (ICE)

The third method applied in this study to predict new toxicity values was the he web-based U.S. EPA Interspecies Correlation Estimation program (U.S. EPA, 2007). ICE models predict acute toxicity values based on estimates of relative sensitivity between the species of interest and that of a surrogate species. They are least square regressions that predict acute toxicity of a chemical to a species for which toxicity data are lacking (the predicted taxon) from the known toxicity of the chemical to a species for which test data are available (the surrogate species; (Dyer et al., 2006). The ICE models were developed by pairing every species with every other species by common chemical from an extensive database. Three or more common

chemicals per pair were required for inclusion in the analysis. For each species pair, Dyer et al. (2006) used a linear model to calculate the regression equation

$$\log(EC_{50\,predicted}) = a + b \cdot \log(EC_{50\,surrogate}) \quad (4)$$

where *a* is the intercept and *b* is the slope of the regression. Only models that gave a significant relationship (p-value < 0.05) are included in Web-ICE. The web-based program allows the median toxicity values and their 95% confidence interval to be calculated for unknown taxa. If the toxicity of a chemical for the same predicted species could be estimated by more than one surrogate species, the weighted mean of the predicted toxicity values was used for calculations (see Appendix B)

Acute toxicity values estimated with ICE were extrapolated to chronic values by using the assessment factors derived by Roelofs et al (2003). We only used predicted acute toxicities for species belonging to one of the taxonomic groups used by Roelofs et al. to derive NOECs. A Monte Carlo simulation with 10,000 iterations was performed. As input data for the EC_{50}s estimated with ICE and the $AF_{acute\text{-}chronic}$ lognormal distributions were used to calculate NOECs. These NOECs were used as input to derive new SSDs, making use of non-parametric bootstrapping.

Chemical potency and species vulnerability (P&V)

The fourth and last method applied in this study to predict new toxicity values uses the characteristics of the chemical and the species to estimate toxicity. Jager et al. (2007) developed a method to decompose toxicity data into a contribution of the chemical (potency) and a contribution of the exposed species (vulnerability):

$$EC_{50} = \frac{1}{P_{cA} \cdot V_{iA}} \quad (5)$$

where P_{cA} is the potency of compound c to disrupt site of action *A*, V_{iA} is the vulnerability of species *i* to effects through site of action A. Jager et al.(2007) derived QSARs for P for four different groups of chemicals (non-polar narcotics, photosynthesis inhibitors, organophosphates and carbamates). The vulnerability was derived for 16 species of 5 different taxonomic groups (algae, arthropods, mollusks, fish and protozoa). In the present study, EC_{50}s were estimated for taxonomic groups with unknown acute toxicity, based on P and V. Estimated acute toxicity values were extrapolated to chronic values by using the assessment factors derived by Roelofs et al. (2003). For the derivation of NOECs, we only used predicted acute toxicities for species belonging to taxonomic groups used by Roelofs et al (Roelofs et al., 2003). A Monte Carlo simulation was performed with Crystal Ball consisting of 10,000 iterations. The calculated NOECs were used as input data to derive the new SSD, using non-parametric bootstrapping.

2.4 Data collection

Dutch researchers compiled a priority list of chemicals that may cause environmental risk when sediment is dispersed on land in the Netherlands (Van Noort et al., 2006), based on expected concentrations and data availability. A complete list of the chemicals with the highest priority is given in Appendix C.

Chronic toxicity values as well as the *Kp* of these chemicals were gathered from European Union Risk Assessment Reports (RAR), as far as they were available (European Chemicals Bureau, 2007b). If no RAR was available for a chemical, data were collected from RIVM reports (for references see Table 2.1). A list of the chemicals for which more than 3 NOECs were available is shown in Table 2.1, including their literature references. Acute toxicity data and information on the toxic mode of action (TMoA) were taken from the RIVM e-toxBase (National Institute for Public Health and the Environment, 2007).

If more than one NOEC or EC_{50} for the same chemical and species were available, the following selection criteria were applied:

- Toxicity values for the most sensitive endpoint were chosen.
- In the case of multiple data on the same end-point and species, the geometric mean was used as the input value for the calculation.

Table 2.1: Data and literature references for the investigated chemicals. (TMoA= toxic mode of action, NOECs= number of no-observed effect concentrations, taxa= number of taxonomic groups, EC_{50}= number of effect concentrations of 50%.

Stof	CAS #	TMoA*	Reference	NOECs	Taxa	EC_{50}*	Taxa*
Anthracene	120-12-7	Nonpolar narcosis	(De Bruijn et al., 1999)	3	3	7	5
Cadmium	7440-43-9	-	(European Chemicals Bureau, 2007a)	28	6	2	1
Chlordane	57-74-9	Neurotoxicant: cyclodiene-type	(De Bruijn et al., 1999)	6	3	2	2
Chromium VI	7440-47-3	-	(Crommentuijn et al., 1997)	43	12	1	1
Copper	7440-50-8	-	(Crommentuijn et al., 1997)	40	8	4	2
4,4'-DDT	50-29-3	Neurotoxicant: ddt-type	(De Bruijn et al., 1999)	3	3	75	6
Dieldrin	60-57-1	Neurotoxicant: cyclodiene-type	(De Bruijn et al., 1999)	8	4	37	4
Endrin	72-20-8	Neurotoxicant: cyclodiene-type	(De Bruijn et al., 1999)	3	2	71	5
α-endosulfan	115-29-7	Neurotoxicant: cyclodiene-type	(De Bruijn et al., 1999)	4	4	25	5
α -HCH	319-84-6	Neurotoxicant: cyclodiene-type	(De Bruijn et al., 1999)	6	5	3	2
β-HCH	319-85-7	Neurotoxicant: cyclodiene-type	(De Bruijn et al., 1999)	5	4	0	0
γ-HCH (lindane)	58-89-9	Neurotoxicant: cyclodiene-type	(De Bruijn et al., 1999)	12	7	10	4
Lead	7439-92-1	-	(Crommentuijn et al., 1997)	30	7	2	2
Naphthalene	91-20-3	Nonpolar narcosis	(European Chemicals	4	3	8	4

			Bureau, 2003a)				
Nickel	7440-02-0	-	(Crommentuijn et al., 1997)	15	6	8	5
Pentachloro-phenol	87-86-5	Uncoupler of oxidative phosphorylation	(De Bruijn et al., 1999)	16	10	12	4
Phenanthrene	85-01-8	Nonpolar narcosis	(De Bruijn et al., 1999)	4	3	3	2
Zinc	7440-66-6	-	(Bodar, 2007)	18	6	5	3

*RIVM e-toxBase (http://www.e-toxBase.com; download data: 12/06/2007)

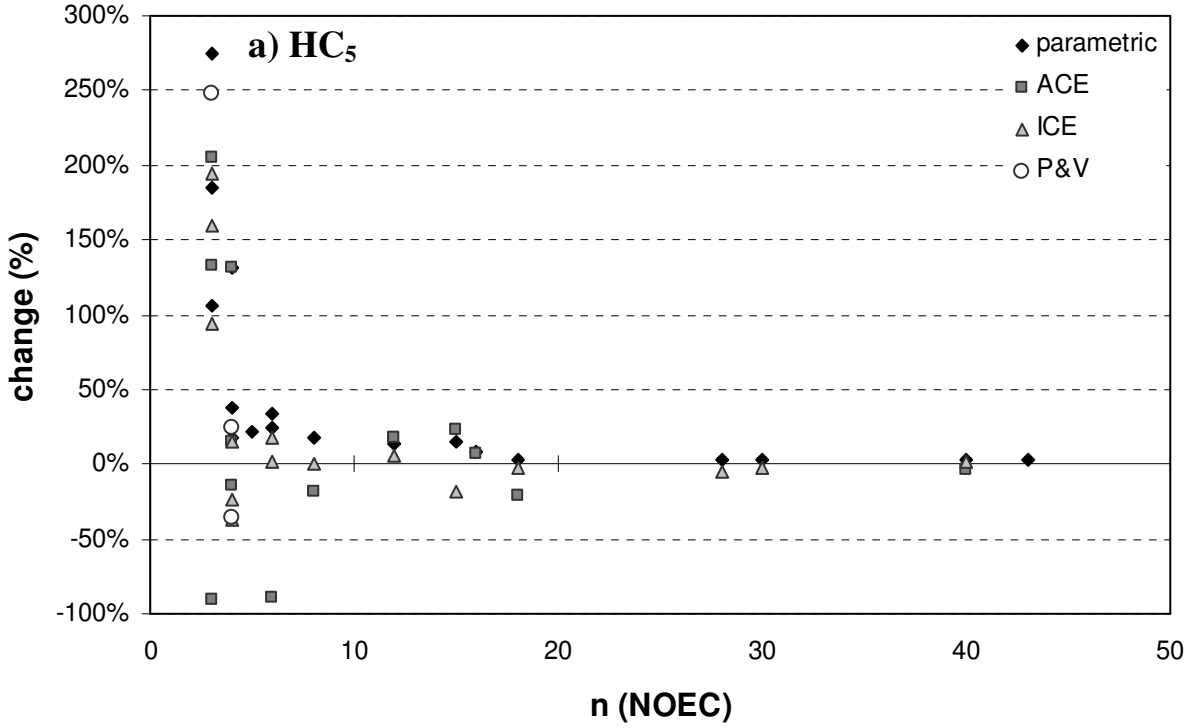
3 Results

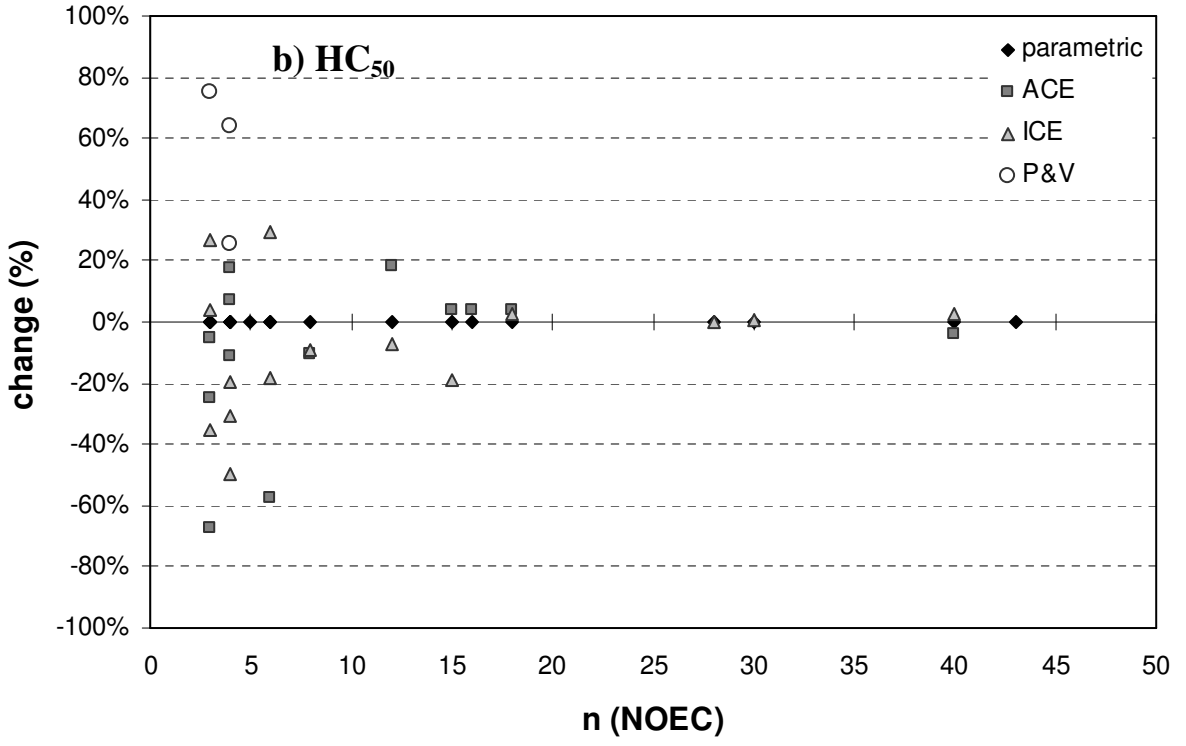
3.1 Change of risk limits

In the present paper, we focus on two different dimensions of changing risk limits: (1) the absolute change in the value of a risk limit, and (2) the probability of an increasing or decreasing risk limit. Table 3.1 shows the probability of the increase of the $EQS_{d\text{-}nd}$ for the four different methods for each chemical. Figures 3.2 a, b and c show the change in the (median) value of the HC_5, HC_{50} and $EQS_{d\text{-}nd}$, respectively, for the different chemicals and estimation methods. A general trend can be seen that the median HC_5 and $EQS_{d\text{-}nd}$ increased whereas the median HC_{50} more or less remained the same after addition. The increase of the HC_5 and the $EQS_{d\text{-}nd}$ was larger for small datasets than for large datasets. For small datasets, the change of the median HC_{50} was more likely to differ from zero than for large datasets. Based on these results, an analysis was performed that resulted in a method which enables the estimation of the change of the risk limits based on the number of chemicals and the variance, which is described in the next paragraphs.

Table 3.1: Probability of the increase of the $EQS_{d\text{-}nd}$ (risk limit that defines the boundary between dispersible and non-dispersible sediment) when using parametric bootstrapping (parametric), acute to chronic extrapolation (ACE), interspecies correlation estimation (ICE) and potency and vulnerability (P&V) to estimate an additional NOEC. (n = number of no-effect concentrations from the original dataset)

chemical	n	parametric	ACE	ICE	P&V
Anthracene	3	74%	61%	75%	98%
DDT	3	74%	21%	81%	-
Endrin	3	74%	71%	60%	-
Naphthalene	4	71%	55%	31%	53%
Phenanthrene	4	71%	54%	31%	76%
α-Endosulfan	4	71%	73%	31%	-
β-HCH	5	70%	-	-	-
Chlordane	6	69%	-	84%	-
α -HCH	6	69%	2%	46%	-
Dieldrin	8	67%	38%	49%	-
Lindane	12	66%	93%	49%	-
Nickel	15	66%	79%	26%	-
Pentachlorophenol	16	65%	65%	-	-
Zinc	18	65%	32%	56%	-
Cadmium	28	65%	-	44%	-
Lead	30	65%	-	53%	-
Copper	40	64%	33%	72%	-
Chromium	43	64%	-	-	-


a) HC5
parametric
ACE
ICE
P&V
change (%)
300%
250%
200%
150%
100%
50%
0%
-50%
-100%
0
10
20
30
40
50
n (NOEC)


b) HC50
parametric
ACE
ICE
P&V
change (%)
100%
80%
60%
40%
20%
0%
-20%
-40%
-60%
-80%
-100%
0
5
10
15
20
25
30
35
40
45
50
n (NOEC)

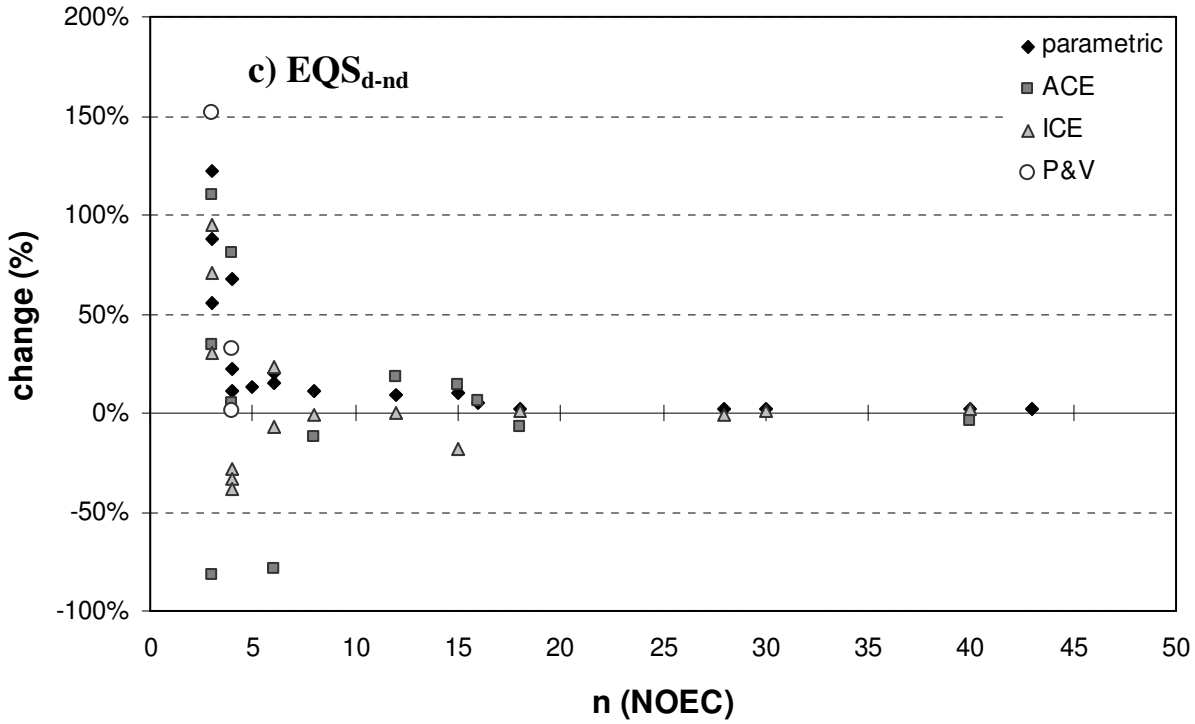


Figure 3.2: Change in the (median) value of the a) HC_5, b) HC_{50} and c) $EQS_{d\text{-}nd}$ plotted against the number of NOECs of the original dataset. A change of 50% implies a 50% increase of the HC_5, HC_{50} or $EQS_{d\text{-}nd}$, whereas a change of -50% implies a decrease of 50%.

When using the parametric bootstrapping method, the median change of the risk limits is always positive, i.e. the risk limits increase. For this method, the change in the median value of the risk limits HC_5, HC_{50} and $EQS_{d\text{-}nd}$ depends only on the number of NOECs of the original dataset and the standard deviation. Because of that, it is possible to predict the new risk limit when the old mean and standard deviation is known. For that purpose, an extrapolation factor d_{50} was derived (for derivation see Appendix D) which enables the prediction of the new median value:

$$\log(HC_p^{m\,\prime}) = \bar{x} - d_{50} \cdot s \qquad [6]$$

where $HC_p^{m\,\prime}$ is the new median hazardous concentration for p% of the species. This d_{50} can be interpreted as an extrapolation factor that enables the user to estimate a new HC_p on the basis of the old mean and standard deviation. The d_{50}s for n=3 to n=50 were derived for HC_5 and HC_{50} and are given in the Appendix D.

In order to illustrate how the HC_5 and the $EQS_{d\text{-}nd}$ changes with n, a factor f_n is derived

$$f_n(HC_5) = \frac{log\left(\frac{HC_{5,\alpha}}{HC_{5,\alpha}^{m\,\prime}}\right)}{log\left(\frac{HC_{5,\alpha}}{HC_{50,\alpha}}\right)} \qquad [7]$$

and analogous for $EQS_{d\text{-}nd}$

$$f_n(EQS_{d-nd}) = \frac{log\left(\frac{EQS_{d-nd,5,\alpha}}{EQS^{m}_{d-nd,5,\alpha}{}'}\right)}{log\left(\frac{EQS_{d-nd,5,\alpha}}{HC_{50,\alpha}}\right)} \quad [8]$$

where $HC^{m}_{5,\alpha}{}'$ and $EQS^{m}_{d-nd,5,\alpha}{}'$ are the median of the $HC_5(\alpha)$ and $EQS_{d\text{-}nd}(\alpha)$ after adding an extra NOEC. For the parametric bootstrapping method, the f_n for each n is constant, whereas the other methods differ from these constants. This is shown in Figures 3.3a and b for α=0.5. A line is fitted through the theoretical f_n to allow a comparison with the other estimation methods. As expected, f_n decreases with increasing *n*.

As can be seen in Figure 3.3, there are a few obvious outliers. For the f_n of the HC_5 these are DDT and α-HCH, derived with the ACE method, and naphthalene and phenanthrene, derived with the P&V and the ICE methods, respectively. DDT and α-HCH are both insecticides. The original dataset did not include NOECs for insects. However, when deriving an additional NOEC the acute toxicity dataset did include EC_{50}s for insects, which were very low compared to the original dataset. As explained in the previous section, naphthalene had a rather low standard deviation. The EC_{50}s estimated with the P&V method were very high. This had a large impact on the standard deviation and the median HC_{50}. The EC_{50}s for phenanthrene estimated with the ICE method were rather low compared to the original dataset of phenanthrene.

For the f_n of the $EQS_{d\text{-}nd}$ the same outliers were found derived by the ACE method. Outliers derived with the ICE method are naphthalene, phenanthrene and α-endosulfan. α-endosulfan is an insecticide as well as an acaricide and very toxic for fish species too. The EC_{50}s estimated with the ICE method were mainly based on toxicity for fish. Therefore, the estimated EC_{50}s were rather low. This lead to a low f_n.

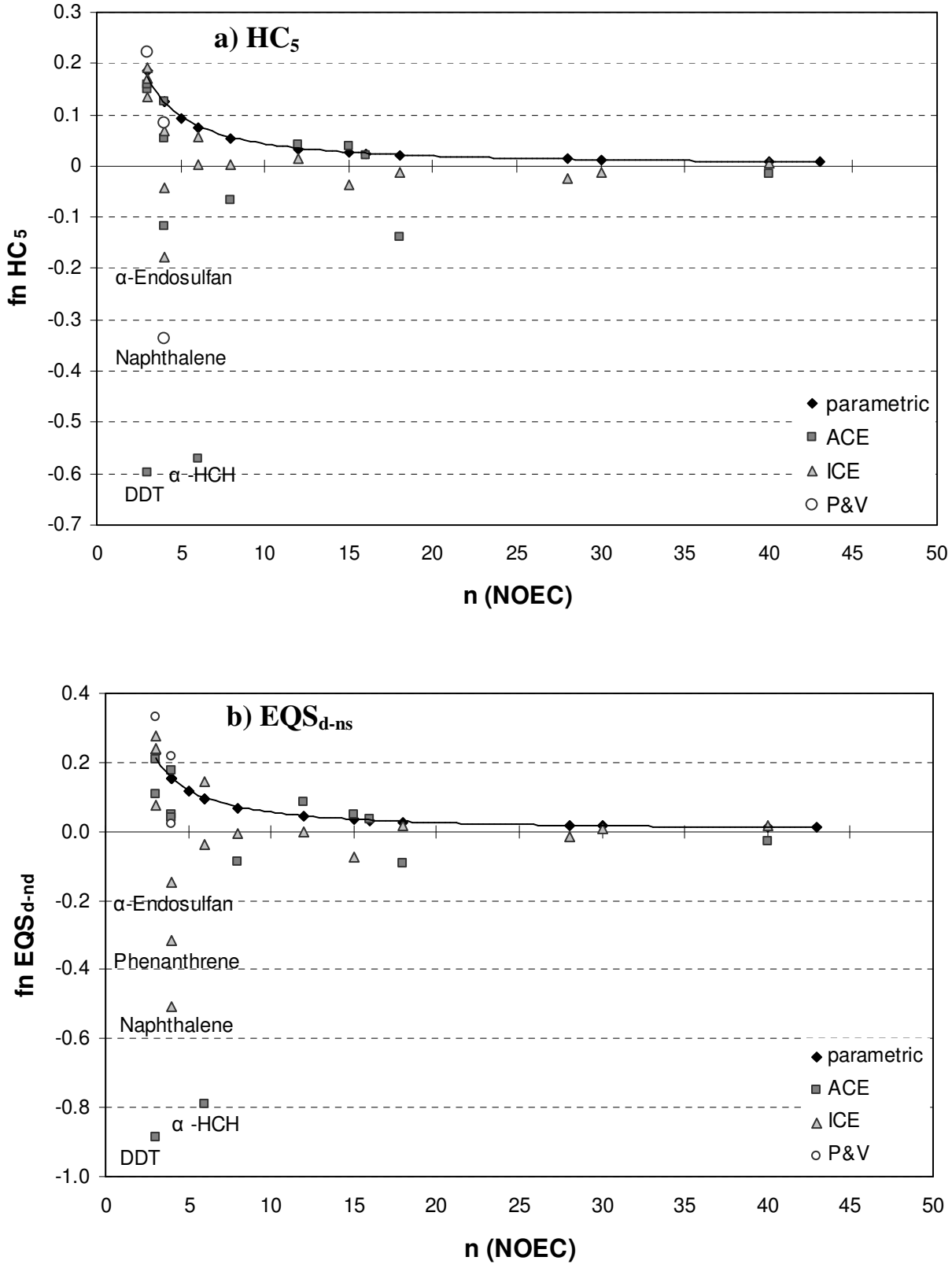


Figure 3.3: The f_n of a) HC_5 and b) $EQS_{d\text{-}nd}$ plotted against the number of NOECs from the original dataset.

Results of the change of the confidence interval of the risk limits are given in Appendix A.

3.2 Volume change

To estimate the potential benefits of adding an additional NOEC to an SSD, the change of the volume of class 3 and 4 sediment was calculated. This was done for 9 chemicals, for which sediment concentrations were available that exceeded the $EQS_{d\text{-}nd}$. Table 3.2 shows the median change of the number of sediment loads belonging to class 3 and 4 and the resulting median volume change. Furthermore, the probability of a decrease of non-dispersible sediments loads is presented in the table. If the probability is more than 50%, it is more likely that the volume will decrease. It can be seen that these figures differ substantially from the figures shown in Table 2. This is due to the fact that the volume change depends not only on the change of the $EQS_{d\text{-}nd}$ but also on the measured concentrations and the number of sediment loads with concentrations above and below the $EQS_{d\text{-}nd}$. If the measured concentrations of a chemical are far above the $EQS_{d\text{-}nd}$, it is very unlikely that the volume will decrease, even if it is likely that the $EQS_{d\text{-}nd}$ will increase. If there are a lot of sediment loads with chemical concentrations below the $EQS_{d\text{-}nd}$, but very close, it is more likely that the volume will increase.

For anthracene it is most likely that an additional NOEC will result in a volume decrease. The same holds for endrin, but because there are only two sediment loads that are above the $EQS_{d\text{-}nd}$, the potential benefits are smaller. According to our results it is impossible that an additional NOEC will result in a volume decrease for chromium, naphthalene and zinc. In the case of chromium and zinc, the sediment concentrations are very high above the $EQS_{d\text{-}nd}$. Even though results showed that it is likely that the $EQS_{d\text{-}nd}$ of chromium and zinc will increase, the increase is too small to result in a decrease of sediment volume. For naphthalene, it is unlikely that an additional NOEC will result in an increased $EQS_{d\text{-}nd}$. Therefore, it is unlikely that the volume will decrease. For the other chemicals, it depends on the estimation method used, whether an additional NOEC will result in a volume increase or decrease. These results show that it is rather difficult to predict beforehand whether an additional NOEC will result in a decrease or increase of the volume of class 3 and 4 sediment.

Tabel 3.2: The original number of sediment loads above and below the $EQS_{d\text{-}nd}$ per chemical and the median change of the number of sediment loads and the sediment volume when making use of parametric bootstrapping (parametric), acute to chronic extrapolation (ACE), interspecies correlation estimation (ICE) and potency and vulnerability (P&V) to estimate new NOECs. The last column gives the likelihood of a decrease in sediment volume.

	# sediment loads		median change of # loads	probability of decrease
parametric	**above $EQS_{d\text{-}nd}$**	**below $EQS_{d\text{-}nd}$**		
anthracene	251	7412	-134	74%
chromium	13	12180	0	0%
copper	162	12063	-1	61%
endosulfan	10	288	-4	67%
endrin	2	334	-2	74%
naphthalene	21	1672	0	0%
nickel	20	12319	-2	60%
phenanthrene	11	10340	-3	67%
zinc	9	12613	0	0%
ACE				
anthracene	251	7412	-112	73%
copper	162	12063	20	32%
endosulfane	10	288	-4	67%
endrin	2	334	-2	71%
naphthalene	21	1672	0	0%
nickel	20	12319	-2	73%
phenanthrene	11	10340	-1	51%
zinc	9	12613	2	0%
ICE				
anthracene	251	7412	-141	74%
copper	162	12063	-1	70%
endosulfane	10	288	4	26%
endrin	2	334	-1	58%
naphthalene	21	1672	2	0%
nickel	20	12319	9	21%
phenanthrene	11	10340	8	29%
zinc	9	12613	0	0%
P&V				
anthracene	251	7412	-178	98%
naphthalene	21	1672	0	0%
phenanthrene	11	10340	-4	74%

4 Discussion

4.1 Estimation methods

It is not the purpose of the present paper to thoroughly discuss the estimation methods used to predict additional NOECs. However, we want to briefly mention that these methods do introduce fundamental uncertainties in the calculations. The parametric bootstrapping method is a strong simplification of reality, which makes use of the assumption that the toxicity for newly tested species will behave according to the distribution of the toxicity for previously tested species. However, it is a very useful method to analyze general trends because of its high predictability. The ACE method states that the ratio of acute and chronic toxicity is constant. However, this ratio can differ greatly for different chemicals and species (Ahlers et al., 2006). Nevertheless, acute to chronic extrapolation can be a suitable method to include as much as possible information in the derivation of EQSs (Duboudin et al., 2004; Roelofs et al., 2003). Therefore, this method has our preference. The ICE method shows how toxicity for one species can be predicted by the toxicity of another species. Unfortunately, no information on the toxicant is taken into account in this estimation (Raimondo et al., 2007). Especially for chemicals with a systemic mode of action this can lead to incorrect results. The P&V method is a rather new method, which shows nicely how information on the chemical as well as on the species can be integrated to predict toxicity. More research is needed to work out this method for different modes of action and species. Although measured data have our preference, we think that these methods show that there are (cheaper) ways to gain a lot of new information by making use of already available knowledge.

4.2 Estimation of potential benefits

The results showed that it is rather difficult to predict whether an additional NOEC will result in a reduction of sediment volume of class 3 and 4. However, several general principles can be identified. First, the change of a risk limit depends on the number of toxicity data used to derive an SSD. The smaller the original dataset the higher the chances that an additional toxicity value will lead to an increase of the risk limit. Furthermore, the increase is higher for small datasets than for large datasets. We have derived a new extrapolation factor, d_{50}, which can be used to predict the change of a risk limit depending on the sample size *n*, based on the mean and standard deviation of the original dataset. Second, the change of risk limits depends on the variance of the toxicity data used to derive an SSD and its relation to the real variance of species sensitivities in an ecosystem. If the variance of the original dataset is very small compared to the real variance, it is likely that an additional NOEC will increase the variance of the sample. When the variance increases, the HC_5 is very likely to decrease. In the present study, this is the case for naphthalene. The change of the HC_{50} also depends on whether the dataset is biased or not, i.e. whether the toxicity values are taken from sensitive or non-sensitive species only, or for a selection of species that is representative for the whole ecosystem. This is especially important for pesticides, which have a specific mode of action. Including target species in the SSD will very likely lead to a decrease of the HC_{50}. In practice, this can be investigated by comparing the dataset to acute toxicity values. Often there are a lot more acute toxicity data available and the variance of the acute data can give an indication of the variance of the chronic data. Third, the change of sediment volume of class 3 and 4 does not only depend on the change of the $EQS_{d\text{-}nd}$, but also on the chemical concentrations in the sediment. If concentrations in sediment loads are

high above the $EQS_{d\text{-}nd}$ it is very unlikely that the volume will decrease. On the other hand, if concentrations are slightly above the $EQS_{d\text{-}nd}$, it is very likely that the volume will decrease.

An additional NOEC can also result in financial benefits. Sediment remediation currently constitutes a problem in the Netherlands because of high remediation costs. Each year 20 million m^3 of fresh water sediment is dredged in the Netherlands, of which almost 40% belongs to class 3 and 4 sediment (Advies en Kenniscentrum Waterbodems, 2001). When we assume the difference in costs for dispersible and non-dispersible sediment to be €30/m^3 and a median sediment load volume of 2625 m^3 (Advies en Kenniscentrum Waterbodems, 2001) that for example for anthracene this means that there is a 50% probability that depending on the estimation method used, between €8.8 and €14 million could be saved by adding one extra NOEC.

4.3 Derivation of EQSs

In the present paper, we made use of the SSD method to derive EQSs. However, according to the EU Technical Guidance Document (European Chemicals Bureau, 2003b) the application of Species Sensitivity Distributions (SSDs) is restricted to situations in which NOECs are available for at least 10 different species of at least 8 different taxonomic groups. Otherwise a different method should be applied which makes use of assessment factors. These factors decrease with an increasing number of available NOECs for up to 3 NOECs. For a dataset of 3 to 9 NOECs the assessment factor remains the same, which means that more data are very likely to lead to more stringent EQSs, but can never result in less stringent EQSs. This is due to the fact that always the lowest NOEC is taken to derive the EQS. As a result money is wasted on measures to meet these conservative EQSs.

For small datasets, the probability that an additional NOEC will result in a lower EQS is very high, whereas for large datasets this probability becomes very small. For example, when deriving an extra NOEC with the parametric bootstrapping method, the probability of a decrease of the MPC (equivalent of the HC_5) for anthracene (3 NOECs) is 26%, whereas for chromium (43 NOECs) this is only 0.01%. These results are opposite to the results of the SSD method, where an additional NOEC is more likely to lead to a less stringent EQS for small datasets as a result of a decrease in uncertainty.

The SSD approach is more in line with the principle that new information should result in less strict safety margins, especially if few data are available. The SSD method is likely to result in less stringent EQSs as more NOECs become available, because of uncertainty reduction. The assessment factor method on the other hand is more likely to result in more stringent EQSs. This makes the assessment factor approach less cost-efficient than the SSD approach.

5 Conclusion

There is no straightforward answer to the question whether including an additional toxicity test in the derivation of an EQS will result in financial benefits. However, we have found general trends and cases in which benefits are likely. For chemicals with a small available dataset, which have standard deviations that are representative for the real standard deviation of the ecosystem and have sediment concentrations that are close above the original EQSs, it is very likely that adding a NOEC will be beneficial.

The main aim in environmental risk assessment is to give the best possible estimate of chemical risks. For environmental management it is important that the assessment results are certain enough so that cost-effective policy decisions can be made. The SSD method makes it possible to make a decrease of uncertainty visible in the resulting EQSs, which is not the case when using the assessment factor method. Therefore, we think that the SSD method is a useful method to derive EQSs, also – or maybe even especially – for small datasets. When making use of the SSD method, all available information is used to derive an EQS and gaining new data is likely to be rewarded with a decrease of uncertainty and an increase of the HC_5 and $EQS_{d\text{-}nd}$. This also means that the effort of government and industry to invest in research is likely to be rewarded. This fits nicely within the REACH framework, which aims for an integration of government and industry in the risk assessment process of chemicals.

A final remark should be made in this context. The calculations in the present study are based on the assumption that the decision of gaining extra data is independent of the original dataset. If for example the decision to extend the dataset is provoked by the uncertainty in HC_5 or the value of HC_5 based on the original dataset, the analysis in this paper becomes invalid.

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List of abbreviations

ACE	acute to chronic extrapolation
$AF_{acute\text{-}chronic}$	assessment factors for acute to chronic extrapolation
EC_{50}	Effect concentration of 50%
EQS	environmental quality standard
$EQS_{d\text{-}nd}$	limit between dispersible and non-dispersible sediment
HC	hazardous concentration
ICE	interspecies correlation estimation
IV	intervention value
LC_{50}	Lethal concentration of 50%
MPC	maximum permissible concentration
NC	negligible concentration
NOEC	no-observed effect concentration
P	chemical potency
SSD	species sensitivity distribution
V	species vulnerability

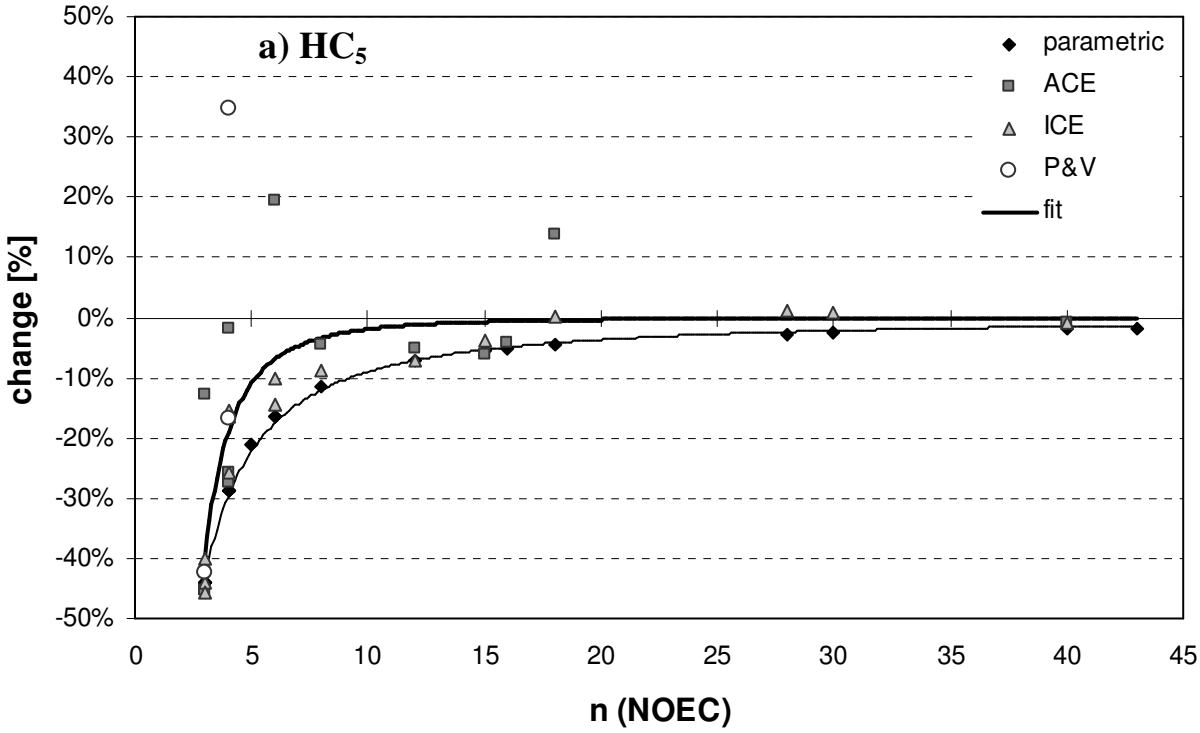
Appendix A

Change of confidence interval

An analysis was performed in order to investigate the impact of an additional NOEC on risk limits for sediment. Figures 3.1 a, b and c show the change of the 90% confidence interval of the HC_5, the HC_{50} and the $EQS_{d\text{-}nd}$, respectively, plotted against the number of NOECs of the original dataset. For all three, the confidence interval decreased in most cases when a NOEC was added. The change is in the same order of magnitude for the HC_5, HC_{50} and the $EQS_{d\text{-}nd}$. The decrease of the confidence interval is dependent on the number of NOECs of the original dataset. For small datasets, the decrease was larger than for large datasets. Clear outliers were naphthalene when calculated with the ICE and the P&V methods, and α-HCH and zinc when calculated with the ACE method. The original dataset of naphthalene had a rather small standard deviation (0.72). Toxicity data of two fish species, one crustacean and one echinoid, were used to derive an SSD. When using the ICE method, 34 EC_{50}s were estimated and used to derive a new NOEC. The variance of the estimated EC_{50}s was much larger. The estimated toxicity for insects was rather low whereas the toxicity for some of the mollusks and amphibians was rather high. This range increased the standard deviation of the SSD and therefore the confidence intervals. In the case of deriving an additional NOEC for naphthalene with the P&V method, the increase of the confidence interval was not the result of a large variance of the estimated data but of very high estimated toxicity values. The estimated NOEC, derived from toxicity data for algae and protozoa, was very high compared to the original dataset, which increased the standard deviation. This shows that for chemicals with a dataset with very little variance it is likely that an extra NOEC will result in an increase of the confidence interval.

The SSD of α-HCH was derived from six NOECs (two algae, one protozoan, one mollusk, one crustacean, one fish). The additional NOEC for α-HCH predicted with the ACE method was derived from three EC_{50}s (one insect and two amphibians). The EC_{50} of this insecticide was very low for the insect (*Cloeon dipterum*). But also the EC_{50} for the two amphibians were rather low compared to the original dataset.

The original dataset of zinc had a standard deviation of 0.997. The additional NOEC for zinc was derived from 5 EC_{50}s (two amphibian, 2 anelida and one protozoa) making use of the ACE method. The standard deviation of the acute dataset was 3.76. The EC_{50} for one of the amphibians (*Rana catesbeiana*) was very high, whereas the other amphibian (*Gastrophryne carolinensis*) had a very low EC_{50}. This resulted in an increase of the variance of the NOECs and in an increase of the confidence interval.


a) HC5
parametric
ACE
ICE
P&V
fit
change [%]
n (NOEC)
50%
40%
30%
20%
10%
0%
-10%
-20%
-30%
-40%
-50%
0
5
10
15
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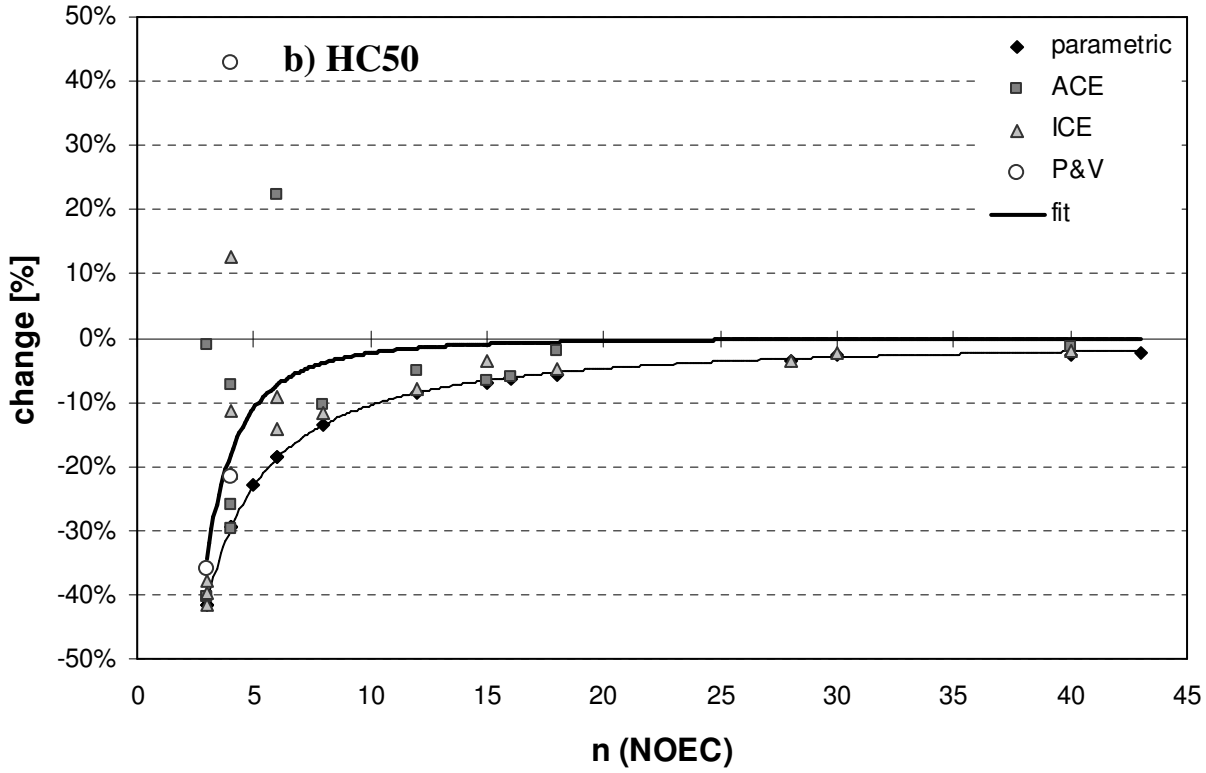
35
40
45


b) HC50
parametric
ACE
ICE
P&V
fit
change [%]
n (NOEC)
50%
40%
30%
20%
10%
0%
-10%
-20%
-30%
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15
20
25
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35
40
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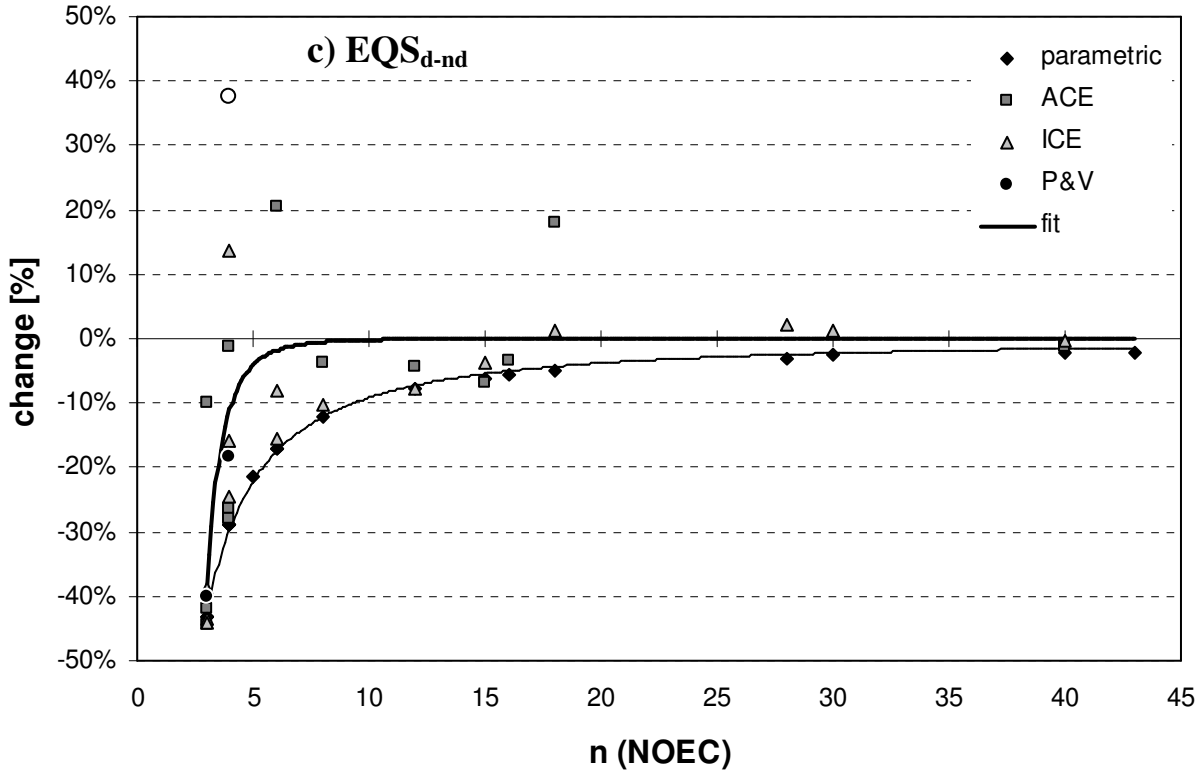

Figure 3.1: Change of 90% confidence interval of a) HC_5, b) HC_{50} and c) $EQS_{d\text{-}nd}$ plotted against the number of NOECs of the original dataset. The fat line is a curve fitted through all data points. The thin line is a curve drawn through the prarametric data points only. The R^2 of the fitted curves through all data points are 0.61, 0.41 and 0.48 respectively.

Appendix B

When making use of the web-ICE model, it possible that the predicted toxicity of one unknown species can be estimated by several known species. In that case the weighted mean $\bar{x}$ of the predicted toxicity values was calculated:

$$\bar{x} = \frac{\sum_i \frac{x_i}{s_i^2}}{\sum_i \frac{1}{s_i^2}} \quad (1)$$

where x_i is the log value of the predicted toxicity and s_i^2 is the variance. The variance was estimated as

$$s^2 = \left(1 + \frac{1}{N} + \frac{(y - \bar{y})^2}{S_{yy}}\right) \cdot MSE \quad (2)$$

where N is the number of predictions, y is the log value of the surrogate toxicity, $\bar{y}$ is the average value of the surrogate, S_{yy} is the sum of squares and MSE the mean square error.

Appendix C

Table 1: List of chemicals with high priority in sediment policy (Van Noort et al. 2006)

Metals	Zinc
	Copper
	Lead
	Nickel
	Chromium
	Cadmium
PHAs	Fluoranthene
	Benzo[a]pyrene
	Benzo[ghi]perylene
	Benzo[k]fluoranthene
	Chrysene
	Benz[a]anthracene
	Indeno[1,2,3-cd]pyrene
	Anthracene
	Phenanthrene
	Naphthalene
Chlorobenzenes	Hexachlorobenzene
Chlorophenols	Pentachlorophenol
PCB	2,2',3,4,4',5-hexachlorobiphenyl
	2,2',4,4',5,5'-hexachlorobiphenyl
	2,2',4,5,5'-pentachlorobiphenyl
	2,3',4,4',5-pentachlorobiphenyl
	2,2',3,4,4',5,5'-heptachlorobiphenyl
	2,4,4'-trichlorobiphenyl
	2,2',5,5'-tetrachlorobiphenyl
Organochloro- pesticides	Endrin
	Aldrin
	Dieldrin
	Telodrin
	Isodrin
	Chlordane
	Hexachlorobutadiene
	4,4'-DDT
	4,4'-DDE
	4,4'-DDD
	2,4'-DDT
	2,4'-DDE
	2,4'-DDD
	α-endosulfan
	Sum α -endosulfan en α -endosulfaat
	α -HCH
	γ-HCH
	β-HCH
	η-HCH
	Heptachlor
	Heptachlor epoxide
Other organic compounds	Mineral oils

Appendix D

Derivation of the extrapolation factor d_{50}

A simulated observation z from the standard normal distribution corresponds to

$$x_{n+1} = \bar{x} + z \cdot s \quad [1]$$

so that

$$\bar{x}' = \bar{x} + \frac{1}{n+1} z \cdot s \text{, and} \quad [2]$$

$$s' = s\sqrt{\frac{n-1}{n} + \frac{1}{n+1} z^2} \quad [3]$$

where x_{n+1} is a new observation drawn from the original dataset. The median of z and z^2 is 0 and 0.45, respectively. This means that the median of the new mean is equal to the original mean, whereas the median of the new standard deviation is smaller than the original standard deviation. If k_s'=ks(FA,α,n+1) then

$$\log(HC_p') = \bar{x}' - k_s' \cdot s' = \bar{x} - \left(k_s' \sqrt{\frac{n-1}{n} + \frac{1}{n+1} z^2} - \frac{1}{n+1} z \right) \cdot s \,. \quad [4]$$

For the median value this can also be written as

$$\log(HC_p^m') = \bar{x} - d_{50} \cdot s \quad [5]$$

The d_{50} includes information on the change of the mean, the standard deviation and the ks. It makes it possible to predict the new risk limit. Table 2 gives a list of d_{50}s for 5, 20, 50, 80 and 95th percentile of the HC_5 and HC_{50}, respectively.

Table 2: The extrapolation factor d_{50} for n=3 to n=50 derived for the 5, 20, 50, 80 and 95th percentile of HC_5 (FA=0.05) and HC_{50} (FA=0.5). (n = sample size)

FA= 0.05	5%	20%	50%	80%	95%
n=2	6.166534	2.88039	1.511705	0.825013	0.451944
n=3	4.52935	2.596843	1.576264	0.979761	0.606924
n=4	3.83996	2.438401	1.600026	1.066736	0.708836
n=5	3.456753	2.336573	1.612041	1.125113	0.784208
n=6	3.209952	2.264697	1.619185	1.168024	0.843036
n=7	3.036055	2.210697	1.623878	1.201387	0.890604
n=8	2.905929	2.168305	1.627175	1.228342	0.930117
n=9	2.804283	2.133931	1.629609	1.250738	0.963641
n=10	2.722295	2.105357	1.631474	1.269748	0.992571
n=11	2.654497	2.081134	1.632945	1.28616	1.017885
n=12	2.597312	2.060269	1.634133	1.300523	1.040291
n=13	2.548293	2.042061	1.635111	1.313237	1.060317
n=14	2.505709	2.025994	1.63593	1.324599	1.078363
n=15	2.468294	2.011683	1.636625	1.334834	1.094742
n=16	2.435103	1.998834	1.637221	1.344121	1.109701
n=17	2.405413	1.987215	1.637739	1.352598	1.123437
n=18	2.378662	1.976643	1.638192	1.360378	1.136112
n=19	2.354403	1.966972	1.638591	1.367552	1.147857
n=20	2.33228	1.958081	1.638946	1.374197	1.158784
n=21	2.312004	1.949872	1.639264	1.380374	1.168985
n=22	2.293335	1.942262	1.63955	1.386137	1.178538
n=23	2.276075	1.935183	1.639808	1.39153	1.18751
n=24	2.26006	1.928577	1.640043	1.396592	1.195959
n=25	2.245149	1.922392	1.640257	1.401356	1.203935
n=26	2.231223	1.916587	1.640453	1.40585	1.211481
n=27	2.218179	1.911124	1.640633	1.410098	1.218635
n=28	2.205931	1.905972	1.640799	1.414123	1.22543
n=29	2.194402	1.901102	1.640952	1.417944	1.231897
n=30	2.183525	1.89649	1.641095	1.421577	1.23806
n=31	2.173242	1.892113	1.641228	1.425038	1.243943
n=32	2.163502	1.887953	1.641351	1.428339	1.249568
n=33	2.154259	1.883993	1.641467	1.431494	1.254953
n=34	2.145474	1.880216	1.641575	1.434511	1.260114
n=35	2.13711	1.87661	1.641677	1.437402	1.265068
n=36	2.129134	1.873161	1.641772	1.440175	1.269827
n=37	2.121519	1.86986	1.641862	1.442837	1.274405
n=38	2.114239	1.866695	1.641947	1.445397	1.278813
n=39	2.107269	1.863658	1.642027	1.447859	1.283061
n=40	2.10059	1.86074	1.642103	1.450231	1.287159
n=41	2.094181	1.857934	1.642175	1.452518	1.291115
n=42	2.088025	1.855233	1.642243	1.454725	1.294938
n=43	2.082105	1.85263	1.642308	1.456857	1.298636
n=44	2.076409	1.85012	1.64237	1.458917	1.302214
n=45	2.070921	1.847698	1.642429	1.460909	1.305679
n=46	2.06563	1.845358	1.642485	1.462838	1.309038
n=47	2.060525	1.843096	1.642539	1.464707	1.312296
n=48	2.055594	1.840907	1.64259	1.466518	1.315457
n=49	2.050829	1.838789	1.642639	1.468275	1.318526
n=50	2.04622	1.836736	1.642686	1.46998	1.321509

FA= 0.5	5%	20%	50%	80%	95%
n=2	1.300371	0.433013	0	-0.43301	-1.30037
n=3	0.983657	0.39946	0	-0.39946	-0.98366
n=4	0.83024	0.364434	0	-0.36443	-0.83024
n=5	0.736591	0.33577	0	-0.33577	-0.73659
n=6	0.670589	0.312497	0	-0.3125	-0.67059
n=7	0.620166	0.293295	0	-0.29329	-0.62017
n=8	0.579819	0.27716	0	-0.27716	-0.57982
n=9	0.546529	0.26338	0	-0.26338	-0.54653
n=10	0.518434	0.251445	0	-0.25144	-0.51843
n=11	0.494301	0.240982	0	-0.24098	-0.4943
n=12	0.473273	0.231715	0	-0.23171	-0.47327
n=13	0.454734	0.223434	0	-0.22343	-0.45473
n=14	0.438226	0.215978	0	-0.21598	-0.43823
n=15	0.423402	0.209218	0	-0.20922	-0.4234
n=16	0.409993	0.203053	0	-0.20305	-0.40999
n=17	0.397787	0.197402	0	-0.1974	-0.39779
n=18	0.386613	0.192196	0	-0.1922	-0.38661
n=19	0.376333	0.18738	0	-0.18738	-0.37633
n=20	0.366835	0.182908	0	-0.18291	-0.36683
n=21	0.358022	0.178741	0	-0.17874	-0.35802
n=22	0.349817	0.174846	0	-0.17485	-0.34982
n=23	0.342153	0.171195	0	-0.17119	-0.34215
n=24	0.334972	0.167763	0	-0.16776	-0.33497
n=25	0.328226	0.164529	0	-0.16453	-0.32823
n=26	0.321872	0.161475	0	-0.16148	-0.32187
n=27	0.315874	0.158585	0	-0.15858	-0.31587
n=28	0.3102	0.155844	0	-0.15584	-0.3102
n=29	0.304821	0.153241	0	-0.15324	-0.30482
n=30	0.299713	0.150764	0	-0.15076	-0.29971
n=31	0.294854	0.148403	0	-0.1484	-0.29485
n=32	0.290224	0.146149	0	-0.14615	-0.29022
n=33	0.285806	0.143996	0	-0.144	-0.28581
n=34	0.281584	0.141934	0	-0.14193	-0.28158
n=35	0.277544	0.139959	0	-0.13996	-0.27754
n=36	0.273672	0.138064	0	-0.13806	-0.27367
n=37	0.269959	0.136243	0	-0.13624	-0.26996
n=38	0.266393	0.134493	0	-0.13449	-0.26639
n=39	0.262965	0.132809	0	-0.13281	-0.26296
n=40	0.259665	0.131186	0	-0.13119	-0.25967
n=41	0.256487	0.129621	0	-0.12962	-0.25649
n=42	0.253423	0.128111	0	-0.12811	-0.25342
n=43	0.250467	0.126653	0	-0.12665	-0.25047
n=44	0.247611	0.125243	0	-0.12524	-0.24761
n=45	0.244851	0.123879	0	-0.12388	-0.24485
n=46	0.242182	0.122559	0	-0.12256	-0.24218
n=47	0.239598	0.12128	0	-0.12128	-0.2396
n=48	0.237095	0.12004	0	-0.12004	-0.23709
n=49	0.234668	0.118838	0	-0.11884	-0.23467
n=50	0.232315	0.117671	0	-0.11767	-0.23232