

LIMITATIONS OF CURRENT RISK CHARACTERIZATION METHODS IN PROBABILISTIC ENVIRONMENTAL RISK ASSESSMENT

FREDERIK A.M. VERDONCK,*† TOM ALDENBERG,‡ JOANNA JAWORSKA,§ and PETER A. VANROLLEGHEM†

†Ghent University, Department of Applied Mathematics, Biometrics and Process Control, Coupure Links 653, B-9000 Gent, Belgium

‡RIVM, Antonie van Leeuwenhoeklaan 9, P.O. Box 1, NL-3720 BA Bilthoven, The Netherlands

§Procter & Gamble, ETC, Temselaan 100, B-1853 Strombeek-Bever, Belgium

(Received 17 September 2002; Accepted 11 March 2003)

Abstract—In probabilistic environmental risk assessment, the likelihood and the extent of adverse effects occurring in ecological systems because of exposure(s) to substances are estimated. It is based on the comparison of an exposure/environmental concentration distribution, with a species sensitivity distribution derived from toxicity data. The calculation of a probabilistic risk can be performed in many ways (e.g., area under the curve in joint probability curves). However, several (hypothetical) examples and some theoretical considerations illustrate that the current risk characterisation methods have an integrative character and they focus on the statistical comparison of two distributions without properly considering the environmental interpretation of these underlying distributions. Several scenarios with varying exposure/environmental concentration distribution and species sensitivity distribution standard deviations are discussed.

Keywords—Joint probability curve Probabilistic risk calculation

INTRODUCTION

The goal of probabilistic environmental risk assessment is to estimate the likelihood and the extent of adverse effects toward species as a result of exposure(s) to substances. It is based on the comparison of an exposure/environmental concentration distribution (ECD) with a species sensitivity distribution (SSD) derived from toxicity data. The calculation of a probabilistic risk can be performed in many ways. The overlap between the exposure concentration (EC) and species sensitivity (SS) probability density functions, as well as between the respective cumulative distribution functions, have both been suggested as a measure of this risk (see Solomon et al. [1]). However, such graphical measures of risk are mathematically not correct. The method for specifically calculating this overlap can be implemented in various ways.

Aldenberg et al. [2] compared different methods mathematically and concluded that the discrete summation for the expected risk of Cardwell et al. [3], Van Straalen's ecological risk [4], the numerical integration of risk distribution curves in the Water Environment Research Foundation methodology [5,6], and the area under the curve (AUC) of joint probability curves (JPCs) are all numerically equal to, and may be interpreted as, the risk of some logEC to exceed some logSS, as originally implemented by the probability of failure in reliability engineering. The graphical interpretation of this risk is the AUC of the product of the ECD cumulative distribution with the SSD probability density function or, alternatively, the AUC of the product of the ECD probability density function with the SSD cumulative function.

In this communication we focus on JPCs [5]. Joint probability curves come in two forms: Either as a graph of ECD exceedence against fraction of species affected (cumulative probabilities of SS) or as a graph of fraction of species affected

against cumulative probabilities of EC. The first is called an exceedence profile plot [7] and involves plotting one minus the cumulative probability of the ECD against the cumulative probability of the SSD for any given concentration (as illustrated in Fig. 1). The second JPC curve results from plotting the cumulative probability of the SSD on the ordinate against the cumulative probability of the ECD on the abscissa for any given concentration. The latter JPC plots are called cumulative profile plots [2]. Cumulative profile plot JPCs are somewhat easier to draw and interpret than are exceedence profile plot JPCs, since they only involve cumulative distribution functions. However, each represents the same risk curve, simply visualized in a different way. Both exceedence profile plots and cumulative profile plots are shown here.

The AUC of JPCs can also be considered as a measure of risk. Mathematically it can be shown that these JPC AUCs are equal to the area under the curves in the overlap plots of the ECD, with the SSD attributable to Van Straalen [4], as referred to above. Hence, the AUC of a JPC expresses the same risk of a random exposure concentration to exceed a random SS [2].

An example of an exceedence profile plot is given in Figure 1. The dashed curves represent thresholds between different types of decisions. These thresholds have to be determined by decision-makers, and their position or shape may move depending on the decision to be made. However, currently no quantitative measures exist for these JPC thresholds. Every data point on the JPC can be easily interpreted (e.g., in Fig. 1: for 50% of the time, [or in 50% of the locations], more than 25% of the species will be affected [e.g., a chronic effect on reproduction]), but interpreting and quantifying the entire JPC seems to be more difficult (e.g., in Fig. 1, how acceptable or unacceptable is this particular JPC?).

In this short communication, it will be shown that these current risk characterization methods have the drawback that they focus on the statistical comparison of two distributions

* To whom correspondence may be addressed
(frederik.verdonck@biomath.rug.ac.be).

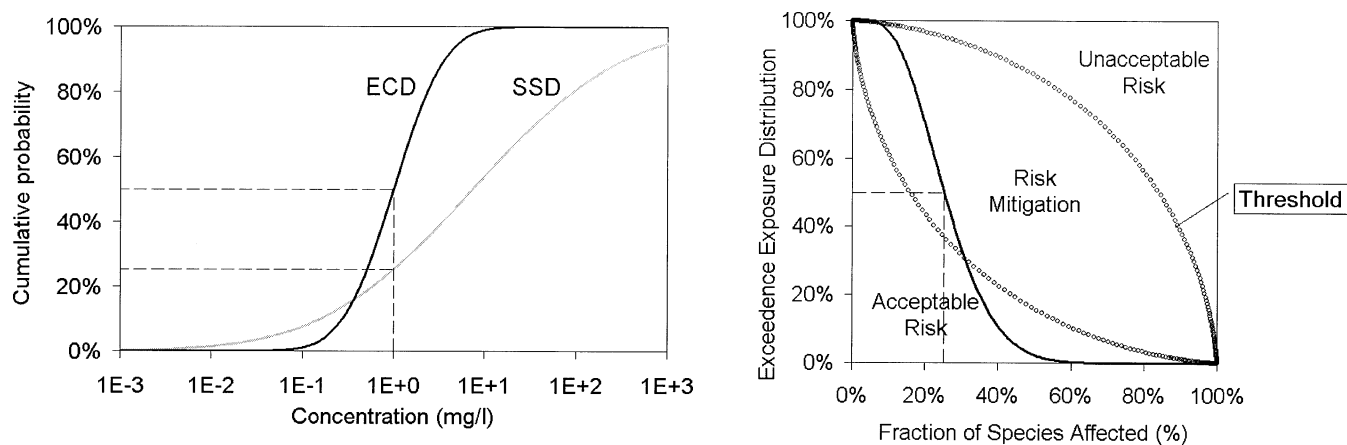


Fig. 1. An example of an environmental concentration distribution ([ECD], left panel), a species sensitivity distribution ([SSD], left panel), and the corresponding joint probability curve (JPC) (exceedence profile plot—JPC and thresholds for acceptance, right panel).

without providing interpretation of the underlying distributions. Important environmental information and interpretation is lost when only the integrative risk is calculated. Theoretical considerations and simulation studies with hypothetical scenarios will illustrate these shortcomings and show that interpretation of the resulting risks should also be carefully made. Depending on the interpretation of the ECD and the SSD, the interpretation of the resulting risk can be totally different.

THEORETICAL CONSIDERATIONS

The probability of some randomly selected EC exceeding some randomly selected SS has been demonstrated to be a common measure of risk [2]. This can be written as

$$\text{Risk} = p(\text{EC} > \text{SS}) \quad (1)$$

where p denotes probability. As described above, several probabilistic risk calculation methods are available. Here, we will show that the probabilistic risk fits well into the paradigm of the deterministic quotient method broadly used in chemical management [8]. The risk quotient (RQ) is an index of risk calculated by dividing an exposure estimate (EC) by a toxicity value (SS). Its properties have been well described [9–11]. The ecological quotient estimates are used to define risks to selected species representing an ecosystem. A critical value of the RQ may form the basis for regulatory action, including possible collection of more information or completion of a more refined analysis [12].

In a probabilistic framework, however, EC and SS are regarded as random variables having probability distributions rather than point estimates. As a result, the RQ will also have a probability distribution. The probability of EC exceeding SS (this probability can be considered as a measure of risk of adverse effects) is equal to the probability that the quotient EC/SS becomes larger than one or that $\log_{10}(\text{EC}/\text{SS})$ becomes larger than zero, since

$$\begin{aligned} \text{Risk} &= p(\text{EC} > \text{SS}) = p\left(\frac{\text{EC}}{\text{SS}} > 1\right) \\ &= p\left[\log_{10}\left(\frac{\text{EC}}{\text{SS}}\right) > 0\right] \\ &= p[\log_{10}(\text{EC}) - \log_{10}(\text{SS}) > 0] \end{aligned} \quad (2)$$

Logarithmic transformations were made because the risk can be easily calculated analytically when lognormal distributions

are assumed for the ECD and the SSD. The result of a quotient of two lognormal distributions (EC and SS) is again a lognormal distribution. But it is much easier to work with the difference of two normal distributions ($\log_{10}\text{EC}$ and $\log_{10}\text{SS}$), because its parameters can easily be calculated. The difference of two independent normal distributions is also a normal distribution with parameters (based on Burmaster and Bloomfield and Verdonck et al. [9,13], see also Fig. 2).

$$\mu_{\log(\text{EC}/\text{SS})} = \mu_{\log(\text{EC}) - \log(\text{SS})} = \mu_{\log(\text{EC})} - \mu_{\log(\text{SS})} \quad (3)$$

$$\sigma_{\log(\text{EC}/\text{SS})} = \sigma_{\log(\text{EC}) - \log(\text{SS})} = \sqrt{\sigma_{\log(\text{EC})}^2 + \sigma_{\log(\text{SS})}^2} \quad (4)$$

with μ and σ indicating the mean and standard deviation of the \log_{10} -transformed data, respectively.

Note that $\mu_{\log(\text{EC}/\text{SS})}$ is not the risk. It is the mean of the $\log(\text{RQ})$ distribution (see Fig. 2). Rather, the risk of some randomly selected EC exceeding some randomly selected SS (see Eqn. 2) is given by the probability of $\log_{10}(\text{EC}/\text{SS})$ exceeding 0. This is equal to one minus the cumulative probability of the above $\log(\text{RQ})$ distribution for $\log_{10}(\text{EC}/\text{SS}) = 0$ or $\text{EC}/\text{SS} = 1$ (see Eqn. 2, also shown in Fig. 2). This calculated risk is equal to the AUC of a JPC [2].

The formula for the probabilistic risk in the case of two normal distributions is

$$\begin{aligned} p(\log \text{EC} - \log \text{SS} > 0) &= 1 - \Phi_{\mu_{\log \text{EC}} - \mu_{\log \text{SS}}, \sqrt{\sigma_{\log \text{EC}}^2 + \sigma_{\log \text{SS}}^2}}(0) \\ &= \Phi_{0,1}\left(\frac{\mu_{\log \text{EC}} - \mu_{\log \text{SS}}}{\sqrt{\sigma_{\log \text{EC}}^2 + \sigma_{\log \text{SS}}^2}}\right) \end{aligned} \quad (5)$$

where $\Phi_{m,s}(x)$ is the cumulative normal distribution of x with mean m and standard deviation s . This is a consequence of Equations 3 and 4, given earlier. In the second panel of Figure 2, the cumulative log risk quotient distribution is visualized. The exceedence (reverse cumulative) log risk quotient distribution is

$$1 - \Phi_{\mu_{\log \text{EC}} - \mu_{\log \text{SS}}, \sqrt{\sigma_{\log \text{EC}}^2 + \sigma_{\log \text{SS}}^2}}(\log \text{RQ})$$

This risk formula clearly illustrates the limitations discussed in the *Introduction*. When the difference between the mean EC and the mean SS is fixed, then interchanging the two standard deviations does not change the risk. In other words, a small ECD variance and a large SSD variance yield the same risk as that found after exchanging the variances but keeping the same means. However, the interpretation of this could differ, as discussed below.

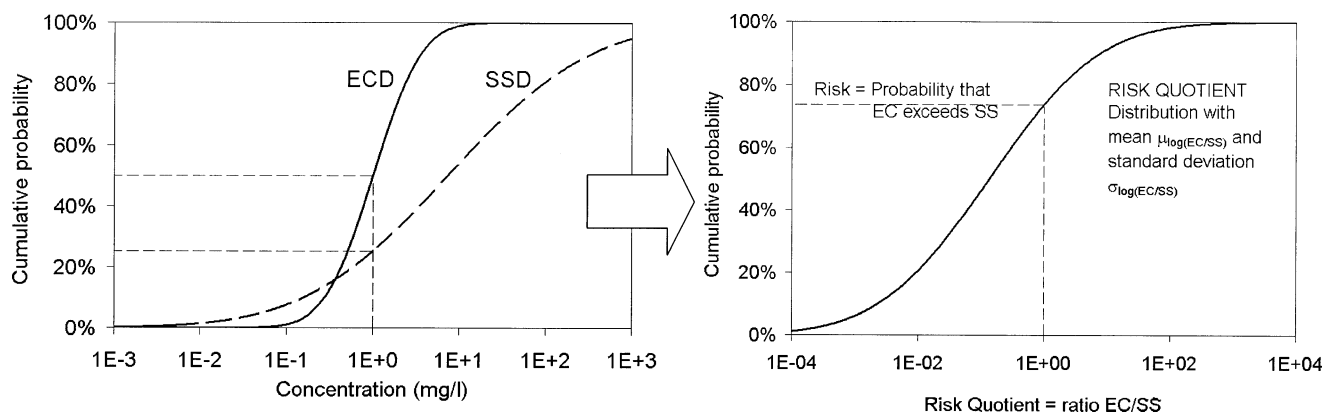


Fig. 2. Calculation of the risk quotient distribution (as a ratio of the environmental concentration [EC] and species sensitivity [SS]) and the risk (right panel) based on the environmental concentration distribution [ECD] and the species sensitivity distribution [SSD], left panel on log scale). The risk is found as one minus the cumulative probability for the ratio = 1 (here, 26%).

The RQ method has the advantage of being easy to calculate for lognormal distributions. If the ECD or SSD has a probability distribution that differs from the lognormal one, the risk has to be calculated numerically (e.g., by means of a Monte Carlo analysis). This is not dealt with here, since this will not influence the conclusions.

Two comments should be made at this point. First, an important condition for using these formulae is that the EC and SS are independent variables. This is generally considered to be the case. Second, in order to assess the quotient of EC and SS, both sets of values have to be compatible [2]. One should not compare 96-h toxicity test endpoints with hourly fluctuating concentrations at a discharge point. The resulting probabilistic risk cannot be interpreted. Instead, either 1-h toxicity tests or, for example, weekly fluctuating concentrations should be used. The time interval of EC measurements or simulation results should be equal to (or larger than) the time interval of SS toxicity testing.

PRACTICAL SIMULATION STUDY

An overview of several hypothetical scenarios can be found in Table 1. In each scenario, the statistical and environmental interpretations are described.

The three rows in Figure 3 show the ECD, SSD, and JPCs from the three scenarios. In each scenario, the risk is an identical 50%. The same results are obtained when using table 5.3 from Aldenberg et al. [2], which tabulates probabilistic risks by only varying the mean and standard deviation of the

log(ECD) relative to the log(SSD). Clearly, the three scenarios represent different environmental situations and should lead to different managerial decisions. This is because environmental effects may differ substantially depending on the interpretation of the ECD or SSD.

To illustrate this dependence on interpretation, a distinction can, for example, be made between an ECD representing temporal variability and an ECD representing spatial variability. When the ECD represents the temporal variation at one monitoring location, scenario 2 (small temporal EC variance, large SS variance) produces a better environmental outcome than scenario 3 (large temporal EC variance, small SS variance), because in scenario 3, almost all species will die approximately 50% of the time. In scenario 2, approximately 50% of the species will die all of the time, but the other 50% might survive. When the ECD represents the spatial variation of a chemical, scenario 3 (large spatial EC variance, small SS variance) will arguably lead to a better environmental outcome than scenario 2 (small spatial EC variance, large SS variance), because in scenario 3, all species will die in approximately 50% of the geographical locations, while in the other 50% of geographical locations, no species are likely to die. In scenario 2, approximately 50% of all species will die at all locations, leading to lower overall biodiversity.

To further illustrate this dependence on interpretation, a distinction can, for example, also be made between a SSD representing acute toxicity and a SSD representing chronic toxicity. In both interpretations, scenario 2 (small temporal EC

Table 1. Overview of the scenarios for the simulation studies (environmental concentration distribution [ECD], environmental concentration [EC], species sensitivity distribution [SSD], species sensitivity [SS], lognormal distribution [LN])

Scenarios	ECD ^a	SSD ^a	Statistical interpretation	Environmental interpretation
1	LN (0, 1)	LN (0, 1)	Same mean for EC and SS Same variances for EC and SS → ECD = SSD	Same distribution for EC and SS
2	LN (0, 1)	LN (0, 5)	Same mean for EC and SS Small variance for EC Large variance for SS	Small range in temporal or spatial EC Very sensitive and very insensitive species (large range)
3	LN (0, 5)	LN (0, 1)	Same mean for EC and SS Large variance for EC Small variance for SS	Large range in temporal or spatial EC All species have more or less the same sensitivity

^a Lognormal distribution with parameters mean and standard deviation of the log-transformed data.

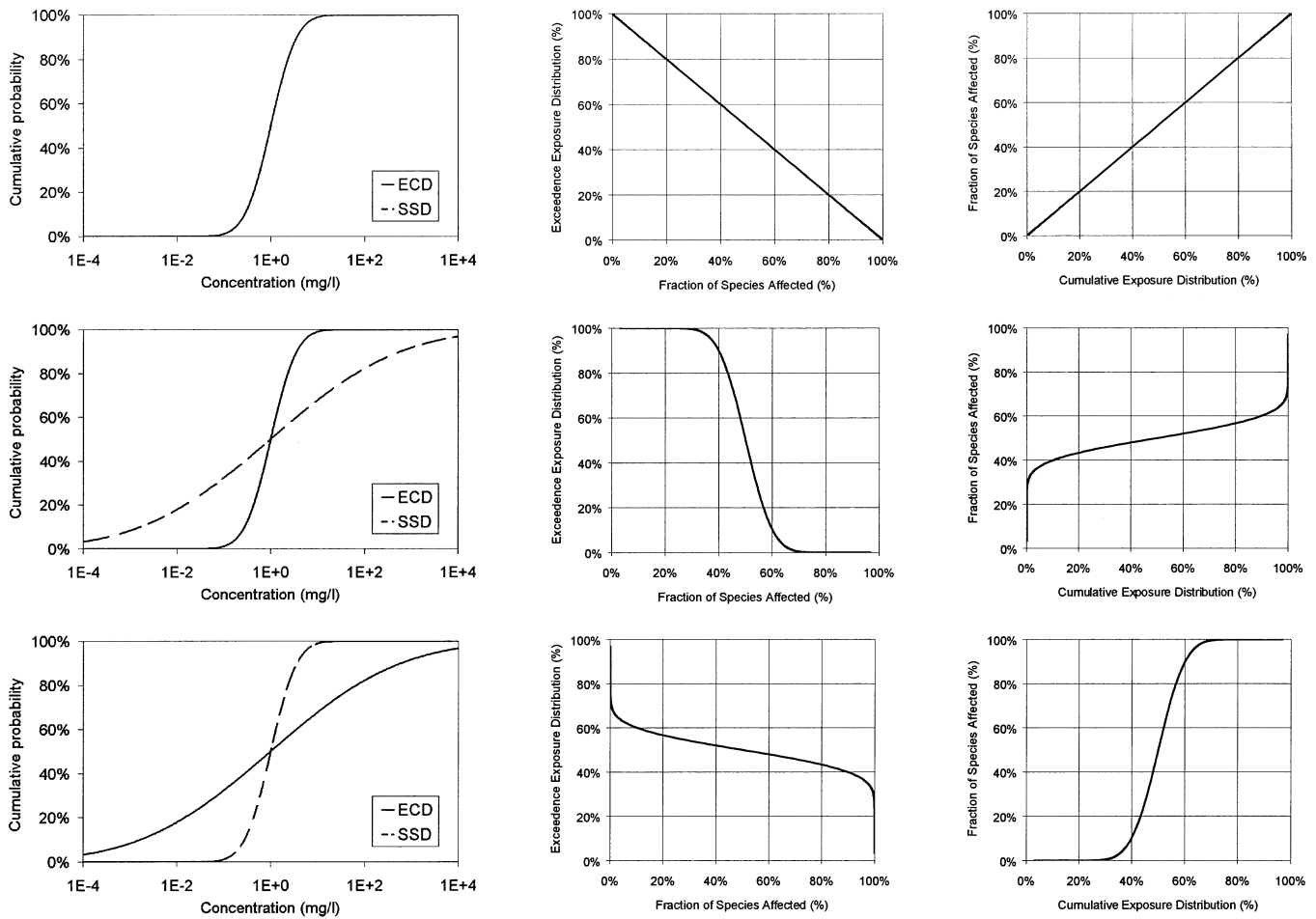


Fig. 3. Simulation results: The first column shows the environmental concentration distribution (ECD) and species sensitivity distribution (SSD) (on log scale), the second column visualizes the joint probability curve (JPC) (exceedance profile plot), and the third column visualizes the JPC (cumulative profile plot); first row: scenario 1, second row: scenario 2; and third row: scenario 3.

variance, large SS variance) produces a better environmental outcome than scenario 3 (large temporal EC variance, small SS variance), because in scenario 3, almost all species will have adverse effects (either acute or chronic) approximately 50% of the time. In scenario 2, approximately 50% of the species will have adverse effects (either acute or chronic) all of the time, but the other 50% will not.

This difference in interpretation of the risk in the different scenarios is also reflected in the shape of the JPC (middle and right column of Fig. 3). Probabilistic risks are, like deterministic risks, only comparative measures. Information on the type of risk and the underlying data needs to be considered for proper interpretation. This may be an advantage of probabilistic methods when compared to deterministic risk calculation, since probabilistic methods are more transparent.

In Figure 4, five JPCs are shown, all of which result in the same risk (12%). However, it is not straightforward to determine JPC thresholds. It has been shown above that, depending on the interpretation of the ECD (and SSD), one JPC may be concluded to be better or worse than the others (even though they have the same risk). Because of the integrative nature of risk calculation, information leading to interpretation is lost.

Clearly, risk is a summary statistic, an integrative measure of the JPC that does not capture all aspects of the shape of the JPC. A potential solution would be to include additional JPC shape parameters. Those may be able to differentiate be-

tween several scenarios resulting in the same risk, as discussed above. Just as the mean and variance are enough to characterize a normal distribution, means and variances of both ECD and SSD must be sufficient to calculate any shape parameter to

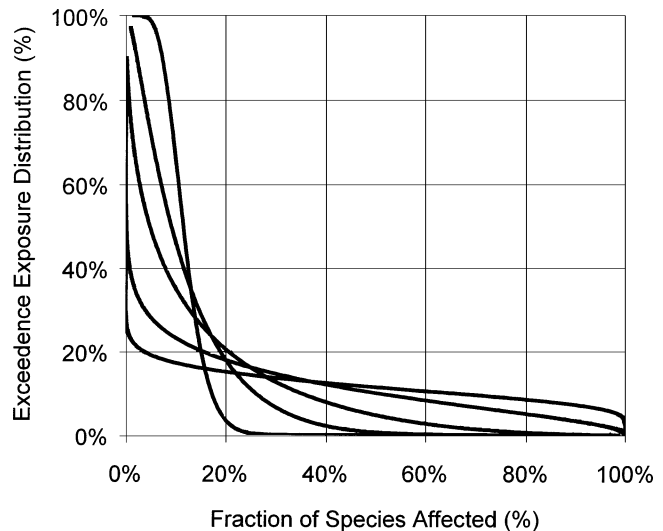


Fig. 4. Several joint probability curves (exceedance profile plots), all resulting in the same risk (12%).

characterize the entire JPC. In order to answer the question "How acceptable or unacceptable is the JPC in Figure 11?," ranges for these shape parameters will need to be determined based on the underlying interpretation of the ECD and SSD.

CONCLUSIONS

Current risk measures, such as the AUC of a JPC, contain insufficient information to account for different environmental circumstances (i.e., different interpretations of the ECD and SSD). Therefore, we recommend that risks always be interpreted from an ecological perspective, forcing the environmental community to compare SSDs with adequate ECDs. Further research is needed on measures additional to the calculated risk that characterize the shape of the JPC and that have an environmental interpretation (depending on the interpretation of the EC and SS) in order to help quantify and manage the risk.

Acknowledgement—This research was funded by a scholarship from the Flemish Institute for the Improvement of Scientific–Technological Research in the Industry. The authors would also like to thank two anonymous reviewers.

REFERENCES

1. Solomon K, Giesy JP, Jones P. 2000. Probabilistic risk assessment of agrochemicals in the environment. *Crop Prot* 19:649–655.
2. Aldenberg T, Jaworska JS, Traas TP. 2002. Normal species sensitivity distributions and probabilistic ecological risk assessment. In Posthuma L, Suter GW II, Traas TP, eds, *Species Sensitivity Distributions in Ecotoxicology*. Lewis, Boca Raton, FL, USA, pp 49–102.
3. Cardwell RD, Brancato MS, Toll J, DeForest D, Tear L. 1999. Aquatic ecological risks posed by tributyltin in United States surface waters: Pre-1989 to 1996 data. *Environ Toxicol Chem* 18:567–577.
4. Van Straalen NM. 2002. Theory of ecological risk assessment based on species sensitivity distributions. In Posthuma L, Suter GW II, Traas TP, eds, *Species Sensitivity Distributions in Ecotoxicology*. Lewis, Boca Raton, FL, USA, pp 37–48.
5. Solomon KR, Takacs P. 2002. Probabilistic risk assessment using species sensitivity distributions. In Posthuma L, Suter GW II, Traas TP, eds, *Species Sensitivity Distributions in Ecotoxicology*. Lewis, Boca Raton, FL, USA, pp 285–314.
6. Warren-Hicks WJ, Parkhurst BR, Butcher JB. 2002. Methodology for aquatic ecological risk assessment. In Posthuma L, Suter GW II, Traas TP, eds, *Species Sensitivity Distributions in Ecotoxicology*. Lewis, Boca Raton, FL, USA, pp 345–382.
7. Giesy JP, Solomon K, Coats JR, Dixon KR, Giddings JM, Kenaga EE. 1999. Chlorpyrifos, ecological risk assessment in North American aquatic environments. *Rev Environ Contam Toxicol* 160:1–129.
8. European Union. 1995. Environmental risk assessment of new and existing substances. Technical Guidance Document. Brussels, Belgium.
9. Burmaster DE, Bloomfield LR. 1996. Mathematical properties of the risk equation when variability is present. *Human Ecological Risk Assessment* 2:348–355.
10. Rai SN, Krewski D, Bartlett S. 1996. A general framework for the analysis of uncertainty and variability in risk assessment. *Human Ecological Risk Assessment* 2:972–989.
11. Campbell KR, Bartell SM, Shaw JL. 2000. Characterising aquatic ecological risks from pesticides using a diquat dibromide case study. II. Approaches using quotients and distributions. *Environ Toxicol Chem* 19:760–774.
12. Warren-Hicks WJ, Moore DRJ. 1995. *Uncertainty Analysis in Ecological Risk Assessment*. SETAC, Pensacola, FL, USA.
13. Verdonck FAM, Jaworska J, Janssen CR, Vanrolleghem PA. 2002. Methodologies to determine risk of chemicals in rivers under data uncertainty. E21472a. *Proceedings, IWA 3rd World Water Congress, Melbourne, Australia, April, 7–12, 2002*.