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The use of Probability Bounds Analysis for Characterising and Propagating Uncertainty in Species Sensitivity Distributions

W.J. Dixon

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Abbreviations

ANZECC – Australian and New Zealand Environment and Conservation Council

ARI - Arthur Rylah Institute for Environmental Research

ARMCANZ - Agriculture and Resource Management Council of Australia and New Zealand

CDF – Cumulative Density Function

DPI – Department of Primary Industries (Victoria)

DSE - Department of Sustainability and Environment (Victoria)

EC05 - Effective Concentration 5%: the concentration of a toxicant that results in a 5% effect

ECD - Environmental Concentration Distribution

ECDF – Empirical Cumulative Distribution Function

LOEC - Lowest Observed Effect Concentration

LOEL - Lowest Observed Effect Level

NOEC - No Observed Effect Concentration

PBA – Probability Bounds Analysis

PDF - Probability Density Function

SSD - Species Sensitivity Distribution

Abstract

This report describes the application of Probability Bounds Analysis (PBA) to the characterisation and propagation of uncertainty in Species Sensitivity Distribution (SSD) models. While a number of previous approaches have sought to analyse some aspects of uncertainty in SSDs, a major limitation of the methods used to date is that they have not incorporated uncertainty estimates propagated from the original toxicity data. By focusing on the use of scalar summaries of effect, such as the No Observed Effect Concentration (NOEC), which by definition are uninformative about uncertainty, previous methods have either described uncertainty as a lack of fit of an assumed model or applied extrapolation techniques that are based on untested assumptions. In this report it is suggested that percentile type summaries, such as Effect Concentrations (EC) or Lethal Concentrations (LC) are better suited to SSD modelling because their associated confidence intervals can be used to describe and propagate uncertainty estimated directly from the original toxicity data. Through the application of PBA it is shown that these confidence intervals can be used to derive bounds on an SSD and subsequent risk estimates.

Contents

Acknowledgments

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1 Introduction

The Species Sensitivity Distribution (SSD) approach to modelling the effects of toxicants forms a key component of environmental regulation and other chemical risk assessment practices throughout the world (ANZECC & ARMCANZ 2000; Posthuma *et al.* 2002b; van Straalen & van Leeuwen 2002). While SSD modelling has generally been considered a useful approach for ecotoxicological risk assessments (Forbes & Calow 2002; van Straalen 2002a), a number of problems with current techniques have been noted (Suter 1998; Newman *et al.* 2000; Van Sprang *et al.* 2004). Despite widespread acknowledgment of the need for uncertainty analysis in risk assessments (Bailar & Bailer 1999; Aldenberg & Jaworska 2000; Suter *et al.* 2000; Pastorok 2002; Burgman 2005), there have been only a few applications of such techniques in ecotoxicology to date (Aldenberg & Jaworska 2000; Posthuma *et al.* 2002a; Verdonck *et al.* 2002; Van Sprang *et al.* 2004).

Uncertainty in ecotoxicological risk assessments arises from a multitude of sources, including (but not limited to) natural variability in the sensitivity of organisms to toxicants, confounding and modifying factors of toxicity, systematic measurement error, lack of knowledge about toxicity mechanisms, and extrapolating across spatial, temporal and organisational scales (Chapman *et al.* 1996; Chapman *et al.* 1998; Cairns Jr 1999). Uncertainties are also introduced into risk estimates through the methods used and assumptions made in the risk modelling process. Although risk assessments are generally performed under constraints of limited information and resources, their aim should be to predict the full range of values that could possibly occur, given the data available (Goodman 2004). Hence, uncertainty analysis is of central importance in risk assessments to ensure rigour, transparency and success in the management process (Morgan & Henrion 1990; Winkler 1996; Suter *et al.* 2000; Andrews *et al.* 2004; Burgman 2005).

Species Sensitivity Distributions are used to combine information on the toxicity of different species to a hazardous agent in order to make inferences about potential effects on groups of species. They are typically constructed by fitting a cumulative distribution function (CDF) to point estimate summaries of species tolerance data, such as No Observed Effect Concentrations (NOEC) or Lowest Observed Effect Concentrations (LOEC) (Aldenberg & Slob 1993; Posthuma *et al.* 2002a). The distributional shape of an SSD is typically assumed to be log-normal, although other parametric and non-parametric fitting procedures have been applied (Newman *et al.* 2000; Shao 2000; van der Hoeven 2001; Verdonck *et al.* 2001; Newman *et al.* 2002; Wheeler *et al.* 2002).

The risk of exposure to the group of species has been defined as the overlap between the SSD and an Environmental Concentration Distribution (ECD), which models the likelihood that different exposure levels have/may occur. This is also defined as the integral or Area Under the Curve (AUC) of the joint probability distribution of the SSD and ECD (van Straalen & Denneman 1989; Aldenberg *et al.* 2002; Verdonck *et al.* 2002). Another estimate of interest in an SSD is the concentration that corresponds to a lower percentile (often 5%) of the distribution, which is interpreted as the maximum allowable level of exposure that will protect the remaining percentage of species (i.e. 95% protected for the lower 5th percentile). These percentile 'standards' then form the basis for setting environmental guidelines for different chemicals.

Limitations of Current Approaches

Perhaps one of the most significant limitations of current methods arises from the use of scalar values (i.e. NOECs) as summaries of exposure-response distributions. A number of authors have discussed in detail the statistical issues associated with the calculation and use of NOEC/LOEC values and how they can be artefacts of experimental design (Hoekstra & van Ewijk 1993; Suter 1993; Chapman *et al.* 1996; van der Hoeven 1997; Chapman *et al.* 1998; Crane & Newman 2000; Koller *et al.* 2000). Although in practice their use in risk assessments may have been necessary due to the low rate of reporting of other measures of effect, scalar values are uninformative about uncertainty, including variability, in a parameter (Hoekstra & van Ewijk 1993; Chapman *et al.* 1996; van der Hoeven 1997; Newman *et al.* 2000). The consequence of modelling each species' exposure-response as scalar is that uncertainty within the response of a species (or individual) to a toxicant is ignored in risk calculations, even though it is an important consideration if the intention is to predict the range of values over which a species or community could be susceptible to a toxicant. A number of authors have suggested the use of low-end effect concentration (EC%) values as more informative and statistically rigorous alternatives, such as the concentration that causes a 1% (EC01) or 5% (EC05) effect (Chapman *et al.* 1996; de Bruijn & Hof 1997; van der Hoeven 1997; Chapman *et al.* 1998). The use of whole exposure response distributions in risk calculations facilitates more informative uncertainty characterisation and statistical rigour, however there have been only a few applications of these in risk assessments to date (Nayak & Kundu 2001; Englehardt 2004; Dixon 2005, 2007) and the reporting of whole datasets is rare.

A second limitation of current SSD practices involves the statistical and mathematical assumptions in the formulations of risk described above. It has been shown that assumptions of one underlying distributional type, such as the normal or log-normal, rarely hold when applied to multiple data sets (Newman *et al.* 2000; van der Hoeven 2001, 2004). Importantly, discrepancies caused by these assumptions often have the greatest implications for values in the tails of a distribution, which are generally the focus of risk assessments (Hattis 1990; Newman *et al.* 2000). The assumption of independence between parameters in probabilistic calculations is also often untested or invalid, can lead to the underestimation of risks and may be unavoidable in standard applications of Monte Carlo analysis (Ades & Lu 2003; Englehardt 2004; Ferson & Hajagos 2004). The formulation of the risk model as 'closed form' or exact solutions to integral equations is also problematic as it is difficult to expand the model to incorporate other factors, such as modifiers of toxicity or exposure, random effects and population growth rates.

A further limitation of the SSD approach involves treating an exposure-response relationship as a random variable (probability distribution), which may actually be incorrect (Suter 1998; Forbes & Calow 2002; Suter *et al.* 2002; van Straalen 2002b; van der Hoeven 2004). Particular problems with this formulation of the SSD include:

- test species may not represent an unbiased random sample from a larger population of potentially affected species;
- interactions between species are not considered;
- different species are treated as equally important and non-dependent on each other in a community, which may not be true; and
- interpretation of the underlying variability generating mechanisms is ambiguous, as is the interpretation of the differentiable relationship between the PDF and CDF of the SSD (Suter 1998; Suter *et al.* 2002);
- CDFs must be increasing and thus cannot incorporate alternative exposure-response functions (such as hormesis or avoidance);
- the use of percentile standards that is inherent in these approaches (i.e. the concentration that protects 95% or 99% of species) assumes that the loss of some species is acceptable and is uninformative about which species may be affected; and
- the use of SSDs and the focus on changes in the number of species within a community means that effects within populations are ignored.

Despite these limitations it has been argued that the probabilistic interpretation of species sensitivity has some utility in representing variability in responses across species and that it is in the interpretation of the results of such processes that problems arise (Forbes & Calow 2002; van Straalen 2002a).

Previous Approaches to Uncertainty Analysis in Species Sensitivity Distributions

In recognition of the uncertainties involved in extrapolating from a small sample of test species in an SSD to communities with a larger number of species, Aldenberg & Jaworska (2000), and Aldenberg *et al.* (2002) applied a sampling theory approach to deriving confidence intervals for percentiles of the normal distribution. This uses extrapolation factors derived from the non-central t-distribution to relate the number of observations in the sample with the variance of the 'true' population percentile. Lookup tables of the extrapolation factors for 90%, 2-sided confidence intervals are provided for various percentiles of interest (Aldenberg & Jaworska 2000; Aldenberg *et al.* 2002). The authors compared this 'classical' approach with a Bayesian formulation of the same calculation using non-informative prior distributions and concluded that the results were essentially identical (Aldenberg & Jaworska 2000; Aldenberg *et al.* 2002). Although calculations were made for both deriving the concentration hazardous to a percentile of a community and the proportion of species affected at a particular concentration, only 'uncertainty' in the SSD was considered.

In another example, Verdonck *et al.* (2002; 2003) and Van Sprang *et al.* (2004) describe a Monte Carlo approach to estimating uncertainty in probabilistic risk quotients that attempts to account for uncertainty in both the SSD and ECD. In this approach, which is based on NOEC data, successive samples are drawn from both distributions and used to create a density of values for a distribution of risk quotients (Verdonck *et al.* 2002; Verdonck *et al.* 2003; Van Sprang *et al.* 2004). This density can then be used to obtain the likelihood that the risk quotient is equal to one. However, like many non-Bayesian Monte-Carlo methods, these approaches are limited in their treatment of correlations between parameters and do not propagate uncertainty estimated from the original data. Similar Monte Carlo approaches have also been applied in human health risk assessments (Finkel 1995; Brattin *et al.* 1996; Thompson 1999; Andrews *et al.* 2004).

While there are an increasing number of studies that have investigated uncertainties in larger and more complex models of exposure and ecological risk and the ecological aspects of the effects of chemical pollution have begun to be addressed, to date there has been little consideration of uncertainty in the exposure-response relationships within these models. Instead, toxicity information has generally been represented as a scalar toxicity reference value or dose and these techniques have not been applied to SSD (see: Bartell *et al.* 2003; Bates *et al.* 2003; Breton *et al.* 2003; Burmaster & Wilson 1998; Crane *et al.* 2003; Ferson *et al.* 1996; Fogarty *et al.* 1996; Jager *et al.* 2001; Landis 2003; Linkov *et al.* 2001; Merrick *et al.* 2005; Moore *et al.* 1999; Pastorok *et al.* 2003; Regan *et al.* 2002a; Regan *et al.* 2002b).

Application of Probability Bounds Analysis to Uncertainty Characterisation in SSDs

This report focuses on the use of effect percentiles and their associated confidence bounds to characterise uncertainty in SSD models through the use of Probability Bounds Analysis (PBA). PBA is a combination of interval arithmetic and probability theory that provide a rigorous method for propagating uncertainty through calculations (Ferson 2002). In particular, PBA provides solutions to problems involving unknown dependencies between variables and uncertainties in the exact nature of distributions (Ferson 2002; Ferson & Hajagos 2004). The solving of some key computational algorithms and the recent development of software that make use of these techniques (RAMAS RiskCalc) has enabled interval and PBA approaches for working with uncertain numbers to be accessible techniques for use in risk assessments (Ferson 2002; Regan *et al.* 2002a; Regan *et al.* 2002b; Ferson & Hajagos 2004; Regan *et al.* 2004).

Conceptually, PBA might be considered an extension of interval arithmetic. If two uncertain numbers are considered, A and B, defined by the respective intervals $[a_1, a_2]$ and $[b_1, b_2]$, then their sum must lie within the bounds $[a_1 + b_1, a_2 + b_2]$, and their product within the bounds $[\min(a_1b_1, a_1b_2, a_2b_1, a_2b_2), \max(a_1b_1, a_1b_2, a_2b_1, a_2b_2)]$ (Ferson 2002). Similar rules exist for other arithmetic operations and analogous solutions have been found for convolutions of interval-type bounds on whole distributions, referred to as probability boxes (p-boxes) (Yager 1986; Williamson & Downs 1990; Ferson *et al.* 2003). PBA has the particular advantage that it is not necessary to assume (probabilistic) independence between parameters because the resultant bounds encompass the full range of probabilistic dependencies between distributions (Ferson & Hajagos 2004). Because p-boxes can be used to describe non-

parametric regions in probability space, various aspects of model and parameter uncertainty can be included in calculations as assumptions about structure within the box are not required. This means that different types or sources of uncertainty may be propagated using the same method and that the resultant bounds on a variable are the best possible given the information available (Ferson *et al.* 2003; Ferson & Hajagos 2004). PBA does have the limitation, however, that the relative likelihood of values occurring inside or outside the bounds specified is not considered beyond the original derivation of the bounds on the parameters.

There have been very few applications of intervals and PBA techniques in risk assessments of the effects of exposure, and even fewer in ecotoxicology. Regan, Sample and Ferson (2002) applied PBA with an exposure model used to determine soil screening levels for terrestrial wildlife. Risk was expressed as hazard quotients and the species sensitive parameter was represented as a single, minimum toxicity reference value. This study compared PBA with Monte Carlo approaches and showed that significant discrepancies could result from unjustified assumptions of independence between parameters (Regan *et al.* 2002b). In another study Regan, Hope and Ferson (2002) compared two-dimensional Monte Carlo and PBA of a food web exposure model, again using a minimum value toxicity reference value, and found similar underestimation of uncertainties even with two-dimensional Monte Carlo techniques (Regan *et al.* 2002a).

2 Methods

Two datasets were used to describe the application of PBA for characterising and propagating uncertainties in SSD models. The first, given in Table 1, is taken from Dixon (2005) and contains a group of EC05 estimates and associated confidence intervals from a series of experiments on the acute toxicity of 4-Chlorophenol (4-CP) to *Daphnia carinata*. Although this dataset is for a single species, the analysis presented is identical to modelling effects on multiple species based on laboratory data (i.e. with similar effects estimates and confidence intervals). This dataset is used as an example to compare SSD and risk values determined using log-normal distribution fitting, the percentile extrapolation method (described by Aldenberg & Jaworska (2000), and Aldenberg *et al.* (2002)) and non-parametric, bounded p-boxes based on confidence intervals for the EC05 data. A hypothetical normally distributed ECD is used to simulate the effects of exposure and to generate risk predictions for these analyses. This distribution also has some uncertainty around its mean and standard deviation (SD) to show the utility of the methods developed in dealing with uncertainty in all parameters. This ECD is presented as both a mean distribution and an uncertain p-box, with a mean of 1.6 (1.5 - 1.7), and SD of 0.5 (0.45 - 0.55). Best fit parametric probability distributions for the EC05 data were obtained using Minitab version 14. In the PBA method the mean response is modelled as an empirical cumulative distribution function (ECDF) of the mean EC05 estimates, while the bounds on the SSD are a p-box of the combined lower and upper 95% confidence intervals. These distributions were constructed via separate applications of the 'mixture' function in RiskCalc v.4 which returns distributions derived from mixtures of inputs, including scalars, intervals, probability distributions and p-boxes (Ferson 2002) (Note that the 'histogram' function provides an identical result for combinations of scalars and intervals in RiskCalc when the confidence level option is set to zero).

Table 1 EC05 values, 95% confidence intervals, log transformations and sample mean and variance for seven experiments on the acute toxicity of 4-CP to *D. carinata* (Dixon 2005).

Experiment	EC05 (mg/L)	Lwr(95%)	Upr(95%)	log(EC05)
1	1.927	0.7836	2.531	0.2848
2	1.801	0.4935	2.643	0.2556
3	1.093	0.0	2.109	0.03858
4	3.451	0.0	5.127	0.5380
5	3.280	0.9682	4.034	0.5160
6	1.896	1.067	2.465	0.2779
7	1.289	0.0	2.345	0.1102
			mean	0.2887
			SD	0.1868

The second example shows the application of the modelling methods to tolerance data obtained from field surveys and, in particular, how taxonomic uncertainty may be treated using PBA. The dataset, given in Table 2, consists of the salinity sensitivities of pond dwelling freshwater macro-invertebrates in the Werribee catchment in Victoria, Australia (Loyn *et al.* 2006), and was collected as part of a larger investigation of the effects of increasing salinity on a series of wetlands and their associated avifauna.

Salinity tolerance information (minimum, maximum and median salinity tolerances) for each taxon was obtained from the Salt Sensitive Database (Bailey *et al.* 2002). This database summarises information on the salinity tolerance of organisms from a large number of field and laboratory studies. Where multiple records were present for a species or where taxonomic resolution was only to genus or family level, the median for that species or group was used as the tolerance value in the risk model, in order to avoid bias. Likewise, the lower and upper bounds on the risk model were based on the minimum and maximum reported values for each species or group. Field and laboratory data have also been considered together because of the lack of availability of information for each taxon. In this example the main response is modelled as an ECDF of the combined median tolerance values for each species (referred to as the medial response) using the mixture function in RiskCalc. The bounds on this distribution are computed as a p-box of the combined min and max values for the species', also using the mixture function.

In both examples the risk from exposure is calculated as the probability that the ECD exceeds the SSD: the comparison operators ">" and "<", or "<=" and ">=" in RiskCalc give bounds on the chance that one exceeds the other, e.g. $p(ECD>SSD)$. This is equivalent to the chance that one distribution subtract the other is greater/less than zero, e.g. $p(ECD-SSD)>0$ or $p(SSD-ECD)<0$.

The proportion of species affected for a given ECD is calculated separately: use of the "cut" function gives the x-values for a particular percentile of a distribution, e.g. "$x_{0.05}$=cut(*SSD*, 0.05)", and the "alpha" function gives the probability of specified x values, e.g. $p(\text{alpha}(ECD, x_{0.05}))$.

Table 2 Salinity tolerance of pond macro-invertebrates (Werribee, Victoria) from Loyn *et al.* (2006).

Order	Family	Genus/Species	Salinity (mg/L)		
			median	min	max
Ostracoda	Cyprididae	*Candonocypris novaezelandiae*	400	400	400
Cladocera	Daphniidae	*Daphnia carinata*	1106	110	17800
	Chydoridae	*Leydigia sp.*	578	476	680
Copepoda	Cyclopoida	*Mesocyclops notius*	1300	600	2000
Hemiptera	Notonectidae	*Unidentified.*	2312	100	30400
	Notonectidae	*Anisops*	3600	100	30400
	Corixidae	*Micronecta*	2420	100	53800
	Corixidae	*Agraptocorixa*	3600	100	27100
	Corixidae	*Unidentified.*	2900	82	53800
Diptera	Chironominae	*Polypedilum*	751.5	82	5500
	Chironominae	*Chironomus*	1804	82	57400
	Chironominae	*Unidentified.*	3120	337	58000
Oligochaeta	*Unidentified.*		437	108	58000
Platyhelminthes	Turbellaria	*Unidentified.*	1885	400	8000
Nematoda	*Unidentified.*		2120	201	19000
Mollusca	Physidae	*Physa acuta*	3200	400	5800

3 Results

4-CP Toxicity Example

The results of fitting a (log)normal probability distribution to the 4-CP EC05 data (in Minitab v.14) are shown as the blue line in Figure 1. This distribution (normal mean= 0.67, SD= 0.43) was found to be a reasonable fit to the data, having an Anderson Darling goodness of fit statistic of 0.326 and a P-value of 0.412 (>0.05) in a lack of fit test. Using the factor tables given in Aldenberg & Jaworska (2000) the 5th percentile and its extrapolated two sided 90% confidence intervals were calculated to be 0.92289 (0.45036 - 1.3084) mg/L. In order to compare this method with bounds based on the 95% confidence intervals for the EC05 data used here, the same calculation Aldenberg & Jaworska (2000), and Aldenberg *et al.* (2002) used to construct their extrapolation tables was performed using the Univariate procedure in SAS version 9.1 (SAS Institute 2003). This produced the 90% two sided intervals 0.45037 - 1.3084 mg/L, which are in accordance with those above, and 95% two sided intervals of 0.35691 - 1.3754 mg/L (Dixon 2005).

The results of non-parametric distribution and p-box fitting in RiskCalc 4.0 to the mean EC05 values, and their 95% confidence intervals, produced the (black) empirical CDF and (red) p-box shown in Figure 1. The 5th percentile, and the corresponding bounds, of these distributions was 1.0929 (0 - 2.109) mg/L, the mean of which is similar to that found using the extrapolation method, although the intervals are clearly wider. Examination of this difference in the uncertainty (confidence) bounds between the two methods reveals that the width of those obtained using the extrapolation technique is 63% smaller than those estimated using PBA methods, and that the upper bound is 65% lower than the bounds one (Dixon 2005). This corresponds to a considerable underestimation of uncertainty by the extrapolation technique described by Aldenberg & Jaworska (2000), and Aldenberg *et al.* (2002) for this data.

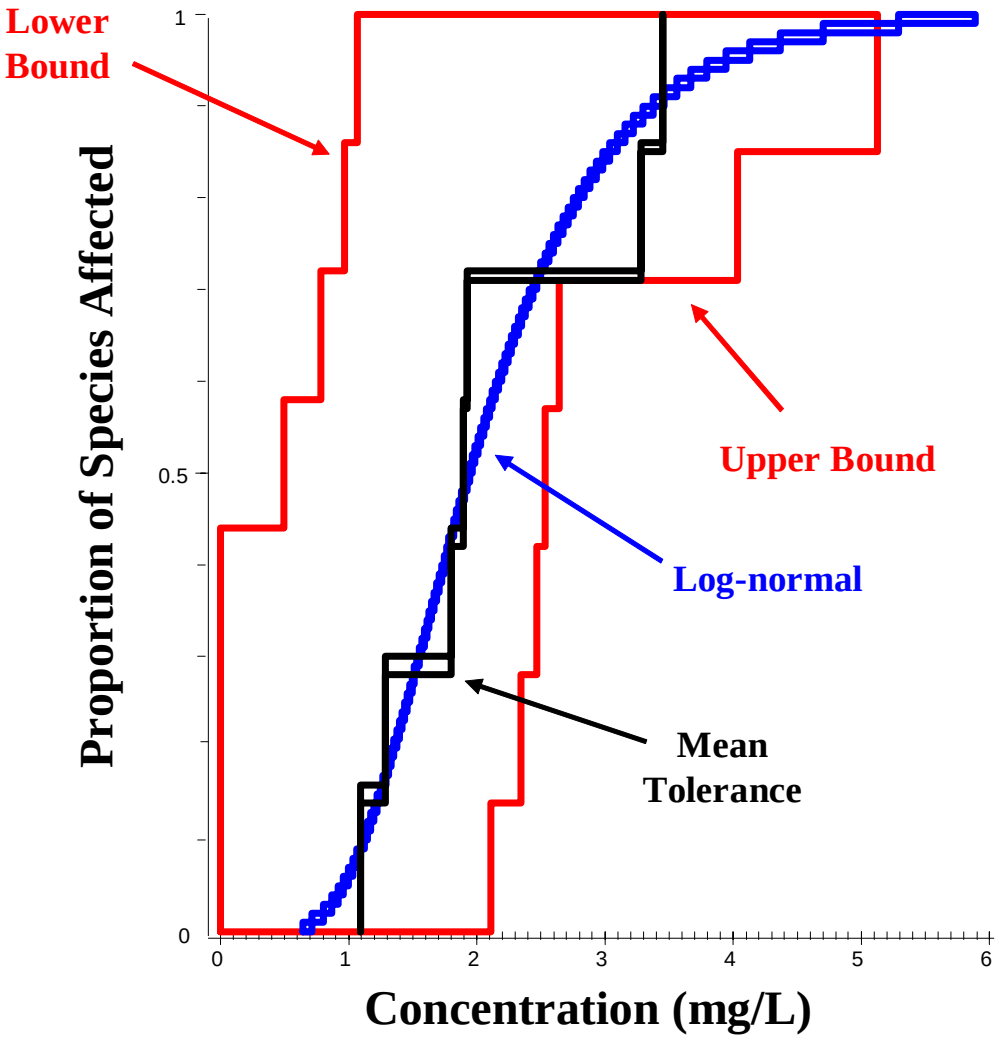

Figure 1 A comparison of different methods for describing SSD models based on EC05 values of the toxicity of 4-CP to *D. carinata*. The blue line is a log-normal distribution and the black line a non-parametric ECDF of the mean EC05 values. The uncertainty bounds on these distributions are represented as a p-box (red lines) derived from the 95% confidence intervals.

Figure 2 compares the three different representations of the SSD with the ECD (green) and its bounds (dark green). Graphically, it can be seen that the red p-box, which describes bounds on the EC05 values, completely overlaps the ECD, indicating that there is at least a 95% chance of an effect from any exposure, based on uncertainty estimated directly from the experimental data. Contrary to this observation, the (log)normal (blue line) and mean ECDF (black line) suggest that exposure of up to 0.6 mg/L should not produce an effect.

Formal calculation of the probability that the SSD is exceeded by the ECD gives the following:

- $p(\text{Mean}_{\text{ECD}} \geq \text{lognormal}_{\text{SSD}}) = 0.74$
- $p(\text{Mean}_{\text{ECD}} \geq \text{ECDF}_{\text{SSD}}) = 0.66$
- $p(\text{Mean}_{\text{ECD}} \geq \text{p-box}_{\text{SSD}}) = 1$
- $p(\text{p-box}_{\text{ECD}} \geq \text{lognormal}_{\text{SSD}}) = 0.80$
- $p(\text{p-box}_{\text{ECD}} \geq \text{ECDF}_{\text{SSD}}) = 0.73$
- $p(\text{p-box}_{\text{ECD}} \geq \text{p-box}_{\text{SSD}}) = 1$

Thus, based on the mean distributions, the lognormal SSD model predicted a higher risk (74%) than the empirical (CDF) of the SSD (66%). Consideration of the bounds on the SSD, however indicated a 100% chance that the lower bound of the SSD (p-box) would be exceeded by the both the mean ECD and its bounds.

Calculation of the chance that 5% of species are affected, given the ECD, results in at least a 90% chance for the lognormal model, 84% for the mean ECDF_{SSD}, 100% for the lower bound and 7% for the upper bound

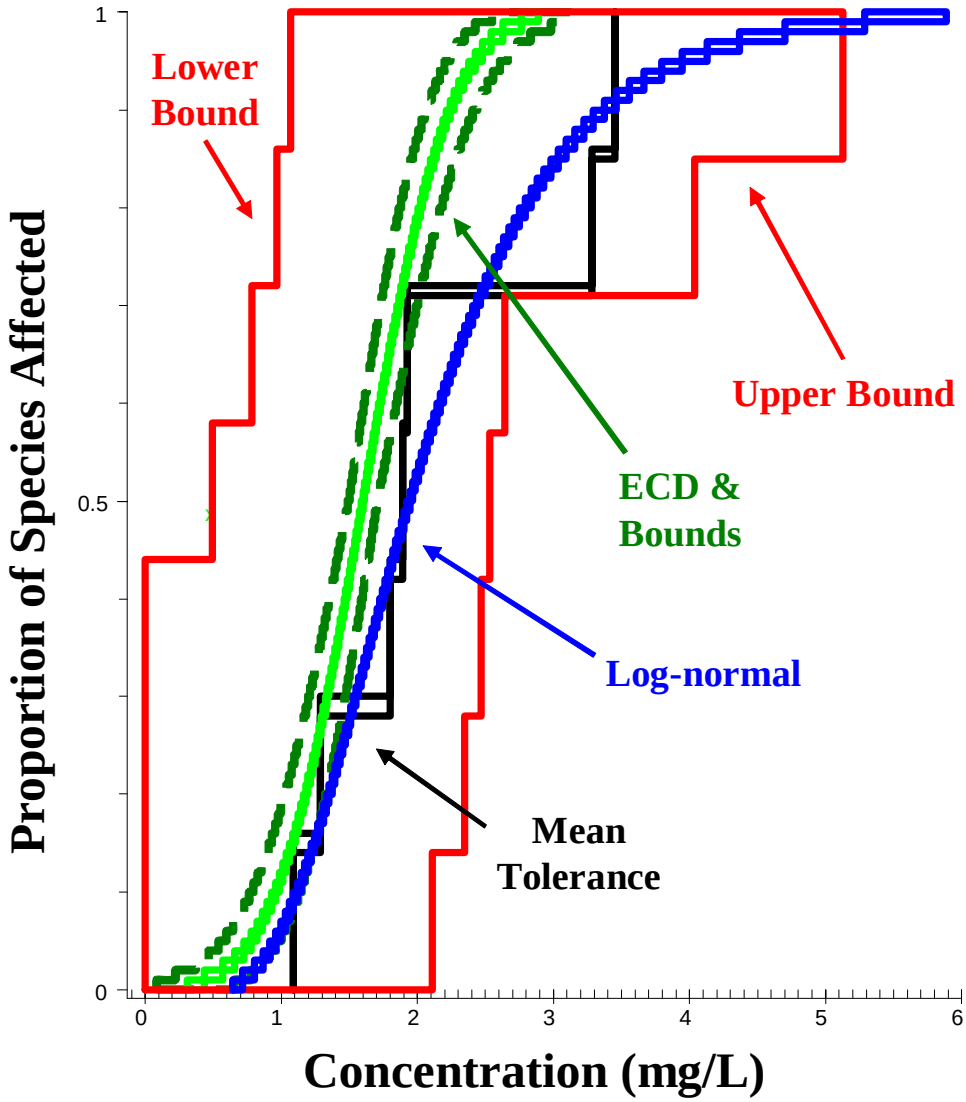

Figure 2 Comparison of the various SSD formulations from Figure 1 (as CDFs) against a normally distributed Exposure Concentration Distribution (green line), shown with uncertainty bounds (dark green dashed lines).

Salinity Field Tolerance Example

Figure 3 shows the results of PBA for the macro-invertebrate salinity data. The medial tolerance SSD (ECDF) is given in black and its upper and lower bounds in red, and is constrained at 10,000mg/L to aid interpretation. The current salinity is presented in blue and the predicted future salinity in green, both as parametric (normal) probability boxes. From this figure and formal calculation of the risk, it was determined that:

- The chance that the medial SSD is exceeded by the current salinity level is 0.27%.
- The future expected salinity level is considerably higher (more than 1,000mg/L) than the medial tolerance for 100% of species;
- The current salinity level exceeds the maximum tolerance bound for 11% of species; and
- The future expected salinity level exceeds the maximum tolerance bound for 17% of species in the SSD.

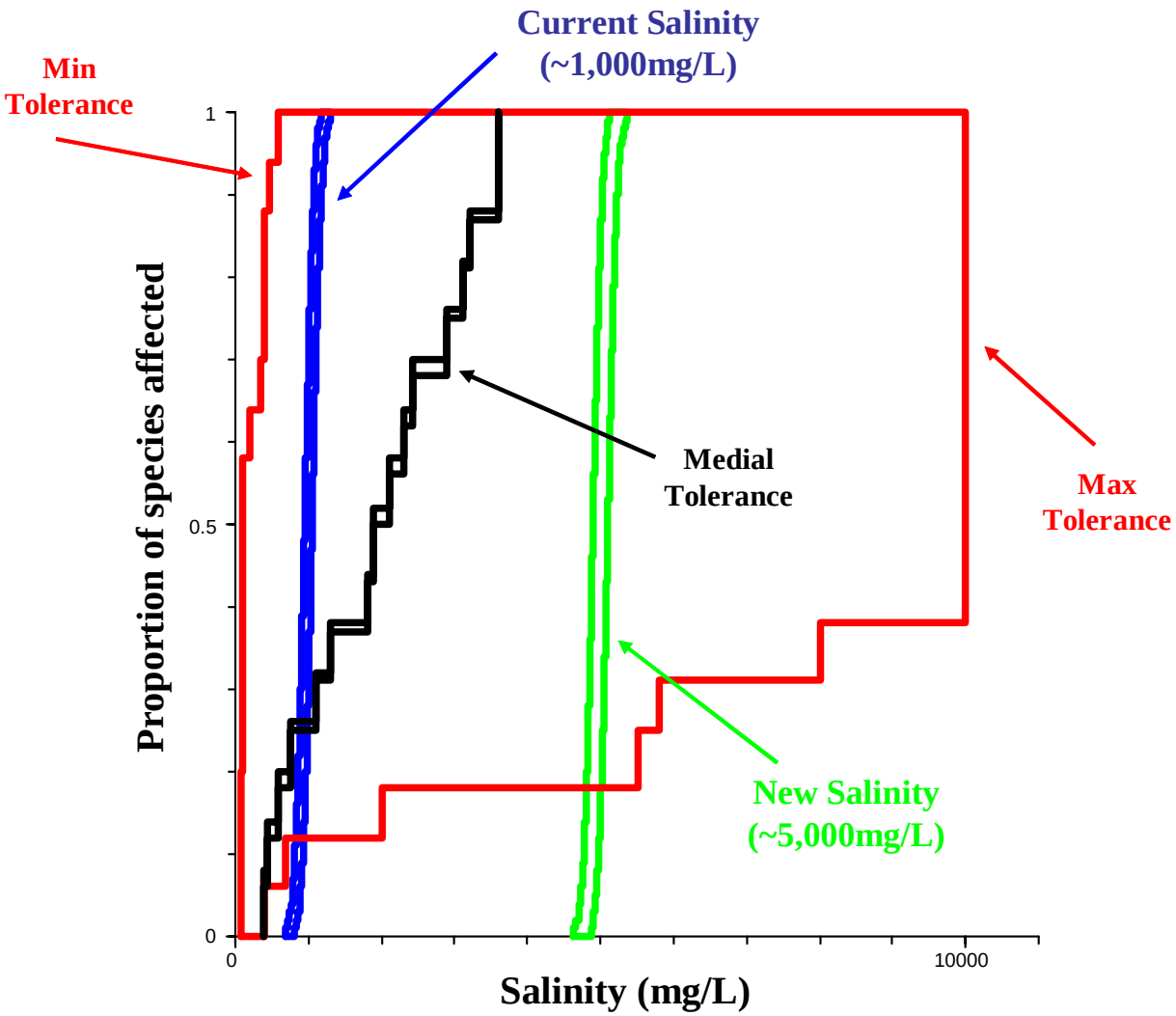

Figure 3 Salinity tolerance SSD for macro-invertebrates in Werribee catchment (constrained at 10,000mg/L), comparing current and predicted exposure distributions.

4 Discussion

One of the major limitations of previous approaches to uncertainty analysis in ecotoxicological risk assessments has been a focus on describing uncertainty as a lack of fit of scalar values to an assumed model, rather than propagating uncertainty estimated from the original data or other available information sources. While a lack of reporting of non-scalar endpoints has contributed to this, the increasing use of other measures of effect, such as EC05, EC10 and whole exposure distributions, means that methods such as those developed here will be required to make full use of the available information.

In the 4-CP toxicity example both the 'standard' parametric (lognormal distribution) and confidence interval extrapolation techniques underestimated risk when compared to probability bounds derived from intervals on the original estimates. In fact, the extrapolation technique described by Aldenberg & Jaworska (2000) was found to underestimate the width of uncertainty intervals by 63% and the upper bound by 65%. While the magnitude of this discrepancy will be dependent on the datasets, this is clear evidence of the inconsistencies and problems associated with extrapolation methods that are based on untested assumptions. It is worth noting also that the results apply to a relatively large, well replicated dataset with low variability. In many risk assessments confidence greater than 95% might be required, further widening the bounds on the risk estimates. Moreover, other sources of incertitude, such as extrapolation from laboratory to field scales of exposure and effect, introduce additional uncertainties into the risk assessment process. While accurate prediction of in situ effects may not be the goal of many risk assessments, quantification of uncertainty is just as important when comparing risks under management scenarios that involve tradeoffs and relative risks.

In the salinity field tolerance example the predicted exposure distribution was found to be above the medial SSD tolerance distribution (i.e. above the reported median for all species). While this appears to indicate a significant effect on the community it was still below the maximum reported tolerance for the majority of the taxa. Additionally, the current exposure distribution is higher than the maximum reported for around 10% of taxa, indicating some of the knowledge gaps and discrepancies of using database sensitivity information. Thus, the actual number of taxa whose maximum tolerance will be exceeded by the expected change in salinity is only 6 or 7 species. While the predicted exceedance of the medial tolerance of all species is a reasonable indication that there might be deleterious effects on the community, consideration of the range of values over which the organisms have been found to occur suggests that the new level may not be outside the tolerance range for the

majority of species. In recognition of the uncertainties involved in this type of risk assessment and the provisional nature of these findings, it was recommended that any changes in salinity that should occur be gradual and regular monitoring and reporting be undertaken in order to detect effects at this time before significant impact may occur.

The SSD modelling techniques described here have the advantage that as taxonomic resolution increases, or better information about the sensitivity of organisms comes to hand, the width of the uncertainty bounds of the tolerance distribution reduce. This method also tackles the question of how to treat sensitivity data when multiple records exist, an issue that can be particularly problematic when dealing with a naturally occurring 'toxicant', as some exposure level may be essential for survival. The use of PBA has the advantage that few distributional assumptions are required and that a number of non-parametric approaches to describing variables are also possible. Treatment of any underlying distributional assumptions is also possible with this method and, unlike many other approaches to this type of risk assessment, it is possible to incorporate uncertainty bounds from any source.

SSD based approaches to risk assessment have many attractive properties, such as being able to extrapolate to community level effects, and, in practice, have provided useful information for managing the effects of chemicals on the environment (Forbes & Calow 2002). However, these and other current approaches used in ecotoxicological risk assessments may have some limitations in their underlying ecological and statistical assumptions. In particular, the notion that the loss of a proportion of species is acceptable, without specific regard to the community structure, which species are expected to be lost or the effect on species' populations, obviously has limited ecological relevance, even in the presence of functional redundancy (Suter *et al.* 2002; van der Hoeven 2004).

5 Summary and Conclusion

This report described the application of alternative methods for characterising and propagating uncertainty in SSDs for ecotoxicological risk assessment. The methods described enable quantification of the bounds on risk estimates, estimation of uncertainty from the original data, propagation of this uncertainty through the risk calculations and quantitative comparisons to be made between risk estimates. In developing these alternative risk models very few assumptions were made about the underlying distribution of parameters and those that were made are easily tested.

The methods described can be easily implemented within current regulatory and risk assessment frameworks for the calculation of both the forward and inverse situations (predicting effects, and setting exposure standards), uses currently available software and provides a non-parametric approach to integrating uncertainty in point estimates into standard approaches. In all cases, confidence bounds on the risk estimates were found to be large compared to either a mean response or standard techniques (including extrapolation). At worst, this finding suggests that underestimation of risk could be commonplace in ecotoxicological risk assessments. At best, it suggests that current approaches to uncertainty analysis are inconsistent. If the goal of the risk assessment process is to predict the true range of values that could possible occur within various practical constraints, then this study clearly demonstrates how uncertainty analysis that makes full use of the available data is essential to the success of the process.

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