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Probabilistic Ecological Risk Assessment Framework for Chemical Substances

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Abstract: The goal of probabilistic ecological risk assessment (PERA) is to estimate the likelihood and the extent of adverse effects occurring to ecological systems due to exposure(s) to substances. It is based on the comparison of an exposure concentration distribution (ECD) with a species sensitivity distribution (SSD) derived from chronic toxicity data. A PERA framework was proposed and illustrated with a case study on the pesticide atrazine in the surface waters of Flanders. The risk and its uncertainty or confidence interval can be visualised in a pie chart. A probabilistic approach results in a more realistic environmental risk assessment and therefore improves decision support of handling impact of individual chemicals.

***Keywords**:* bootstrap; water quality; atrazine

1. INTRODUCTION

Yearly, thousands and thousands of existing and new chemicals are released in the environment. Regulation puts constraints on these chemical emissions and these are based on environmental risk assessment. The goal of a risk assessment is to estimate the likelihood and the extent of adverse effects occurring to humans and ecological systems due to exposure(s) to substances. Environmental risk assessment is based on the comparison of a predicted or measured exposure concentration (EC) with a 'no effect concentration' based on a set of (acute or chronic) toxicity test results. In this deterministic framework, inputs to the exposure and effect prediction models are single values and the risk is calculated as simple ratios of EC and effects.

This approach does not account for uncertainty, spatial and temporal variability of the environmental concentration (EC) and the species sensitivity (SS). Therefore, there is a need for more realistic risk assessment frameworks. In a Probabilistic Ecological Risk Assessment (PERA), the EC and SS are treated as random variables taken from probability distributions (respectively ECD and SSD) which are combined to give a risk distribution. Furthermore, incorporating spatial characteristics of the receiving environment can further increase realism. By geography referencing the risk assessment, the spatial variability is explicitly accounted for in each local risk assessment and as a result the remaining overall variability can be reduced.

In these types of risk assessments, the distinction between data uncertainty and variability must be made. Variability represents inherent heterogeneity or diversity in a well-characterised population. Fundamentally a property of nature, variability is usually not reducible through further measurement or study. Temporal and spatial variations of chemical concentrations can be captured in a variability distribution, called Exposure Concentration Distribution (ECD). Various species sensitivities towards a chemical can also be captured in a variability distribution called Species Sensitivity Distribution (SSD). These distributions are also used in water quality standard setting (e.g. in EU environmental risk assessment practices). In Figure 1, the variability distributions are visualised by a black line. Uncertainty represents partial ignorance or lack of perfect information about poorly characterised phenomena or models (e.g. sampling or measurement error), and can partly be reduced through further research [Cullen and Frey 1999]. In Figure 1, the uncertainty is visualised as a grey band around the cumulative variability distribution function. For each percentile of the variability distribution, an uncertainty or confidence interval can be calculated (i.e. the uncertainty distribution).

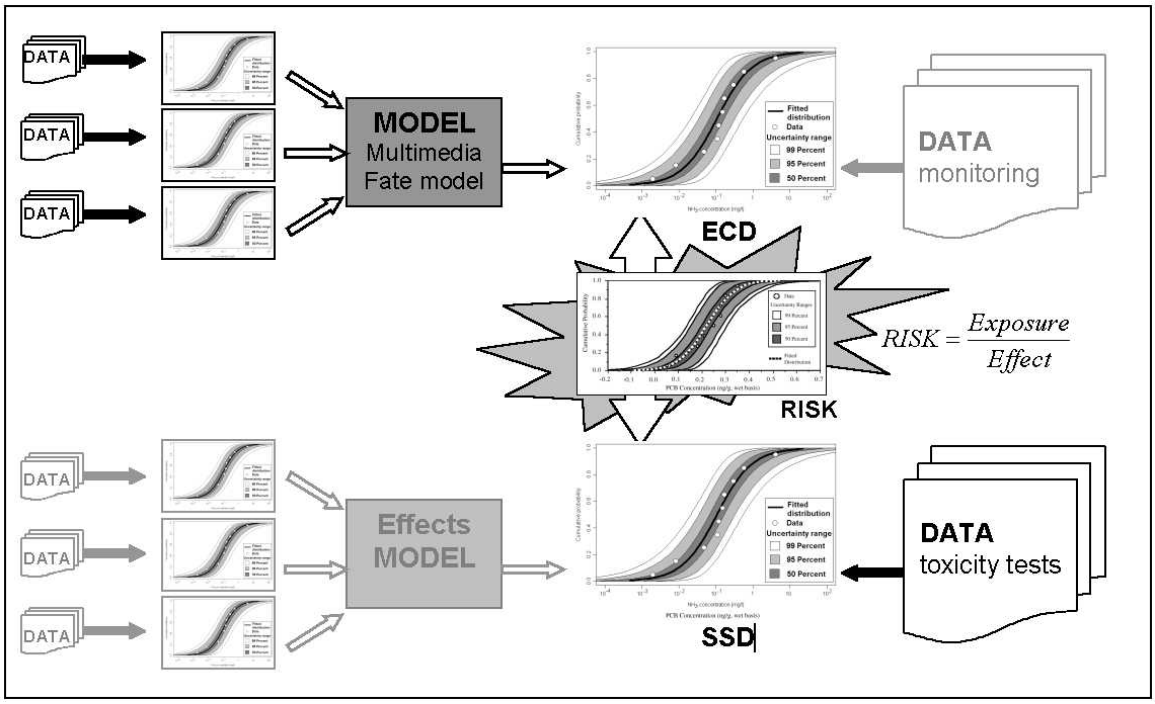

Figure 1. Probabilistic ecological risk assessment (PERA) framework in which data sets are characterised by their variability and uncertainty

The goal of this paper is to perform a more realistic risk assessment by means of existing and new probabilistic tools and models. The outcome of a PERA is a probability of expected risk with an uncertainty interval. Suppose, as an example, that the risk is 30%. A risk manager will feel more confident if he or she knows that the 90% uncertainty interval of that expected risk is between 25 and 35% rather than between 10 and 50%. Also, a proposal will be made of how to visualise and communicate risk in order to improve decision support. A case study on the risk of atrazine in the surface waters of Flanders will be presented to illustrate the framework.

2. PERA FRAMEWORK

Two different approaches can be used to determine the Exposure Concentration Distribution (ECD) and the Species Sensitivity Distribution (SSD). Data from either measurements in the environment or toxicity tests can be used directly (see Figure 1, right side). The alternative is to use prediction or extrapolation models (see Figure 1, left side). However, these models also need (other) data, which are again characterised by uncertainty and variability. As a consequence, a distinction should be made between statistical methods for characterising data uncertainty and variability (full arrows in Figure 1), and methods for propagating uncertainty and variability through mathematical models (open arrows in Figure 1).

In the subsequent sections, the uncertainty and variability characterisation and propagation, and the risk calculation are discussed.

2.1 Variability and Uncertainty Characterisation

One of the important issues to address is how accurate the typically applied statistical techniques (like (non-) parametric bootstrap, Bayesian statistics, and maximum likelihood estimation) are in characterising uncertainty estimates at low sample sizes. Indeed, it was found that these techniques (especially non-parametric versus parametric methods) give different results and, therefore, a comparison was made between them [Verdonck et al. 2001]. A parametric method depends on the assumption of an underlying model (e.g. lognormal distribution). A non-parametric method on the other hand only depends on the data points themselves. The results of Verdonck et al. [2001] indicate that the considered methods display varying robustness and accuracy, especially when sample size decreases. Most of the methods were found suitable to be used with small sample sizes, except for a particular kind of non-parametric bootstrapping where resamples are taken from the empirical distribution function. There was no clear reason to prefer parametric or nonparametric methods. However, the results are very sensitive to the choice of the method.

Here, the numerical bootstrap technique was preferred since the technique is easy to understand and implement. A detailed description of the bootstrapping method can be found in literature [Cullen and Frey 1999]; [Davison and Hinkley 1997]; [Efron and Tibshirani 1993]. Given a data set of sample size n, the general approach in bootstrapping is to assume a (non)parametric distribution, which describes the quantity of interest, to perform r replications (e.g. r = 5000) of the original data set by randomly drawing, with replacement, n values, and then calculate r values of the statistic of interest. For the case study, the lognormal (i.e. a parametric) model was selected.

2.2 Variability and Uncertainty Propagation

A very common sampling method for propagating variability or uncertainty is Monte Carlo simulation. Random samples of model input parameters are selected according to their respective assigned probability distributions. In this way difficulties to estimate model input parameters and taking into account the inherent uncertainty or variability in specific processes are overcome. Once the samples from each input distribution are selected, the set of samples is entered into the deterministic model. The model is then solved as it one would do for any deterministic analysis. The model results are stored and the process is repeated until the specified number of model iterations (shots) is completed. Instead of obtaining a discrete number for model outputs (as in a deterministic simulation) a set of output samples is obtained [Cullen and Frey 1999].

In most current PERA, variability and uncertainty are not treated separately although they are two different concepts. To deal with the issue, a second order or 2-dimensional or embedded Monte Carlo simulation is developed [Burnmaster, 1996], [Cullen and Frey 1999]. It simply consists in two Monte Carlo loops, one nested inside the other. The inner one deals with the variability of the input variables, while the outer one deals with uncertainty. For each uncertain parameter value in the outer loop a whole distribution is created in the inner loop based only on variability. In this way changes in variability-dependent frequency distributions under the influence of parameter uncertainty can be quantified.

2.3 Modelling the Risk Distribution

The characterisation of the risk of toxicants to species, when both EC and SS are variable and uncertain, is the central issue in Probabilistic Ecological Risk Assessment (PERA). The methodology is well developed in literature [Aldenberg et al. 2001]. Among all risk calculation techniques available, one method was selected in this study: the risk quotient method.

2.3.1 When Only Variability is Considered

The probability of exceeding some randomly selected EC exceeding some randomly selected SS can be regarded as a measure of risk [Aldenberg et al. 2001]. This can be written in formulae as:

$$\mathbf{Risk} = \mathbf{P}(\mathbf{EC} > \mathbf{SS})$$

The quotient method is well described in literature [Burmaster and Bloomfield 1996] [Rai et al. 1996]. The ecological quotient estimates are used to define risks to potential ecological receptors. In environmental risk assessment, this risk quotient is an index of risk calculated by dividing an exposure estimate (EC) by a toxicity value (SS). The nominator and denominator values are in the same exposure units (e.g. mg/l) so that the ratio is dimensionless. A critical value of the risk quotient may form the basis for some regulatory action, including possible collection of more information or performing a more refined analysis [Warren-Hicks and Moore 1995].
In a probabilistic framework, the EC and SS are regarded as probability distributions rather than point estimates. As a result, the quotient will also be a probability distribution (see Figure 2 but remove visually the grey bands). The probability of EC exceeding SS is equal to the probability that the quotient EC/SS becomes larger than 1. This probability can be considered as a measure of expected risk of adverse effects. This percentage can also be visualised as a column chart (see Figure 2 but remove visually the grey bands).

When lognormal distributions are assumed for the ECD and the SSD, the risk can be calculated analytically. The result of a quotient of two lognormal distributions is again a lognormal distribution and its parameters can easily be calculated using the following equations (based on Burmaster and Bloomfield [1996] and also found by Aldenberg et al. [2001]):

$$\mu_{Risk} = \mu_{EC} - \mu_{SS}$$

$$\sigma_{Risk} = \sqrt{\sigma_{EC}^2 + \sigma_{SS}^2}$$

with μ and σ respectively the mean and standard deviation of the log-transformed data

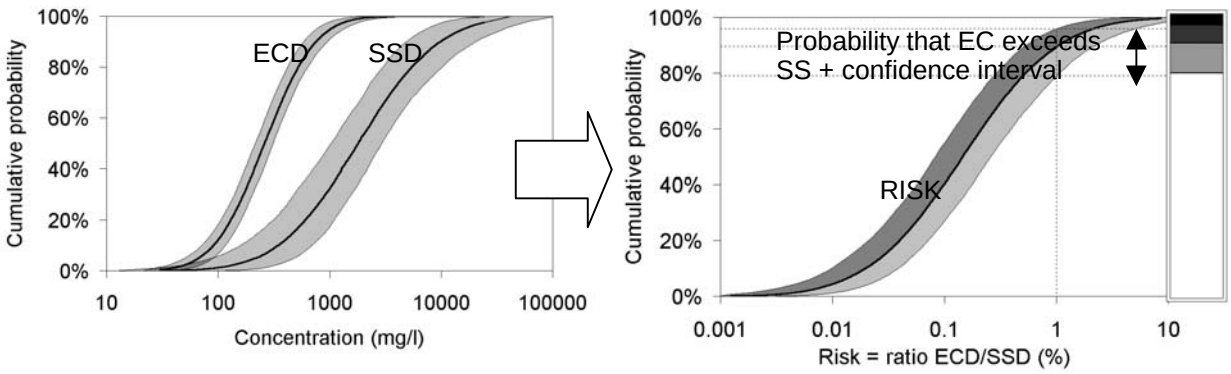

Figure 2. Calculation of the expected risk and its uncertainty interval based on ECD and SSD

In case the ECD or SSD have a different probability distribution, the risk can always be calculated numerically by means of a Monte Carlo analysis.

Two important remarks have to be made. First, an important condition for using these formulas is that EC and SS are independent variables, which is the case. Second, in order to assess overlap of ECD and SSD, both sets of values have to be compatible [Aldenberg et al. 2001]. One cannot compare 96h toxicity tests to hourly fluctuating concentrations at a discharge point. The time interval of EC measurements or simulation results should be equal to (or larger than) the time interval of SS toxicity testing.

2.3.2 When Variability and Uncertainty are Considered

In the previous section, only the variability of the ECD and SSD was considered. This resulted in a risk variability distribution. The ECD and SSD are also uncertain because of sampling error. Adding a Monte Carlo sampling loop to the risk calculation can capture this uncertainty. In each run, an ECD and SSD will be selected from their respective uncertainty bands and the risk distribution will be calculated. After many runs, the risk distribution will also have an uncertainty band (Figure 2).

Remark that other uncertainty issues, not dealt with here, still need to be solved such as lab to field extrapolation uncertainties of the SS, the representativeness of the species in an SSD, model uncertainty, etc.

The risk distribution visualised as a column chart in Figure 2 can also be visualised as a pie chart as in Figure 3. The entire pie represents 100%. The grey shades indicate how large the risk is with a pre-defined certainty. The larger the white slice, the lower the risk is. The more black, the larger the expected risk is. The larger the grey slices are, the more uncertainty there is on the estimated risk. The example shows that the median expected risk is 23% (50% certainty) and there is 95% certainty that the risk is smaller than 45%.

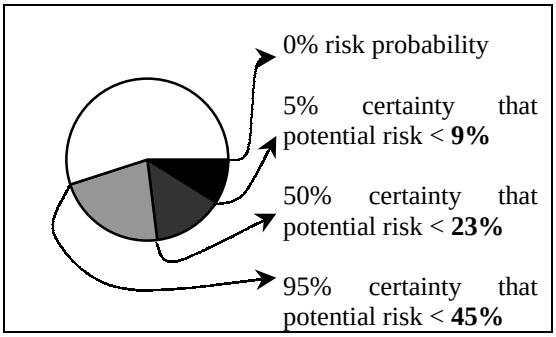

Figure 3. Visualisation of the potential risk of 23% and its 90%-uncertainty interval

3. CASE STUDY

As an illustrative case study, probabilistic risks and their 90%-uncertainty intervals were predicted for the pesticide atrazine in the river catchments of Flanders in Belgium. Since atrazine is such a widely used herbicide and the chemical nature of this compound is persistent, it is considered a great potential for groundwater and surface water contamination. Therefore, it is frequently detected. The greatest risk of atrazine runoff occurs shortly after the application because it hasn't had time to adhere to the soil particles and is still at the surface of the soil [Lipishan and Lee 1996].

The data set for the SSD consists of chronic toxicity values (NOEC: No Observed Effect Concentrations) and can be found in Versteeg et al. [1999]. A lognormal distribution was assumed and fitted to the data. The fit was satisfactory.

The ECs were obtained from the Flemish environmental agency [VMM 2001]. Atrazine was (mostly monthly) measured at 134 locations from 1991 till 2000. Only the reliable data from the years 1997 till 2000 were considered. It is assumed that this monitoring network is representative for all rivers in Flanders. The cumulative empirical distribution function of all the EC is shown in Figure 4. A lognormal distribution was assumed and fitted to the data but the model did not fit very well to the data (see grey curve in Figure 4) because the data are left censored i.e. the value 50 ng/l is frequently observed. This value corresponds with the detection limit of atrazine. Censored data can be handled in different ways. Govaerts et al. [2001] recommends to replace every value below the detection limit with a random number between zero and the detection limit (here 50). After the correction for censoring, the lognormal distribution now fits very well to the data (see black curve in Figure 4). For every monitoring station, a lognormal distribution was fitted to the data. The resulting ECD represents the variation of the concentration (mostly temporal) at that station.

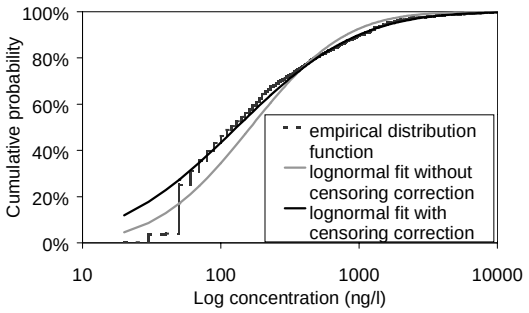

Figure 4. Cumulative probability distribution of atrazine measurements in surface waters in Flanders

4. RESULTS

The results of the local PERA of atrazine for all monitoring stations in the river networks of Flanders are visualised in Figure 5.

The results of the local PERA of atrazine in the basins of Flanders indicate that the predicted atrazine risks are around 1,6% for many monitoring locations. Most of the median risks are smaller than 5% and most of the upper risk 90% uncertainty intervals are smaller than 15%.

5. DISCUSSION

Based on the discussed framework and the results of the case study, one can say that PERA improves transparency and credibility, it focuses data collection, it avoids worst-case assumptions, it improves decision support and, above all, it is more realistic compared to the current deterministic risk assessment approaches. As a result, this approach enables risk managers to evaluate the full range of variability and uncertainty instead of just using point estimates of exposure, effects and eventually risk.

The case study additionally shows that by geography referencing the risk assessment, the spatial exposure variability is explicitly accounted for in each local risk assessment and as a result the remaining overall variability can be reduced.

Visualisation of the expected risk as pie chart promises to be a good communication tool. The darker the slice of the pie chart, the larger the expected risk is. The larger the grey slices are, the more uncertainty there is on the estimated expected risk.

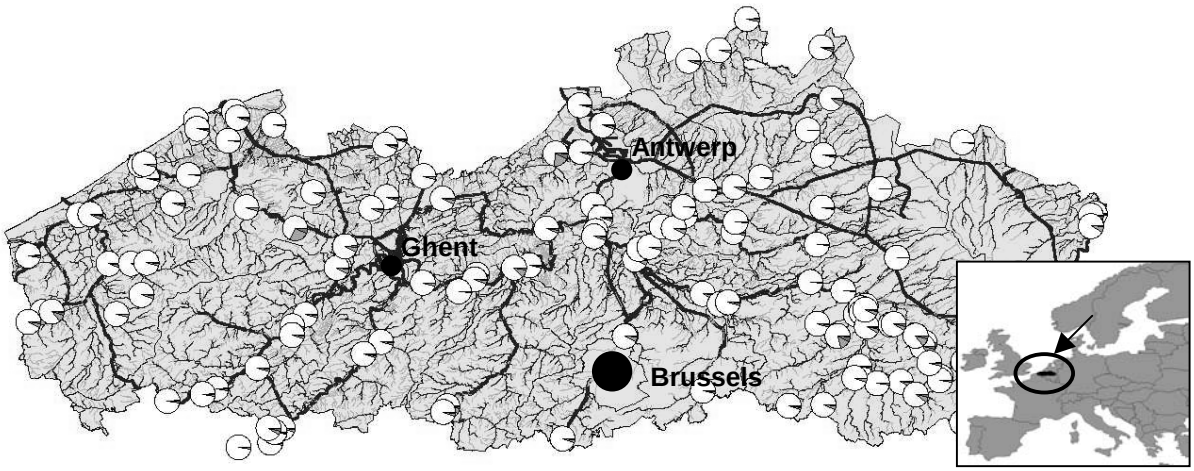

Figure 5. Atrazine risk in the catchments of Flanders (Belgium)

However, the framework can still be further improved. First, the example in Figure 2 shows that the calculated risk is only a comparative measure. Despite the large overlap of the ECD and the SSD, the predicted expected risk is 23%. The tails of the ECD and SSD are very important since the largest EC (like the 95th-percentile of the ECD) will first have effects on the most sensitive organisms (like the 5th-percentile of the SSD). A better risk measure would be obtained when more attention is paid on the upper tail of the ECD and the lower tail of the SSD. Second, geography referencing the risk is only useful when both the ECD and the SSD are geography referenced. In the case study, only the ECD was geo-referenced. The SSD was the same for every location while in reality spatial differences lead to different local SSD's [Janssen et al. in press]. Hot spots could also be found based on the geo-referenced ECD's.

6. CONCLUSION

A framework for performing probabilistic environmental risk assessment (PERA) was proposed and illustrated with a case study. The risk and its uncertainty or confidence interval can be visualised in a pie chart. This uncertainty interval is important for the decision-maker since it expresses how reliable the risk assessment is. A probabilistic approach results in a more realistic environmental risk assessment and therefore improves decision support of handling impact of individual chemicals. Some suggestions for further improvement of the PERA were made: the tails should be considered more in the risk calculation and the effects assessment should also be geography referenced in order to refine the risk assessment.

7. ACKNOWLEDGEMENTS

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