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Using the expert model PERPEST to translate measured and predicted pesticide exposure data into ecological risks

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Abstract

An important topic in the registration of pesticides and the interpretation of monitoring data is the estimation of the consequences of a certain concentration of a pesticide for the ecology of aquatic ecosystems. Solving these problems requires predictions of the expected response of the ecosystem to chemical stress. Up until now, a dominant approach to come up with such a prediction is the use of simulation models or safety factors. The disadvantage of the use of safety factors is a crude method that does not provide any insight into the concentration–response relationships at the ecosystem level. On the other hand, simulation models also have serious drawbacks like that they are often very complex, lack transparency, their implementation is expensive and there may be a compilation of errors, due to uncertainties in parameters and processes. In this paper, we present the expert model prediction of the ecological risks of pesticides (PERPEST) that overcomes these problems. It predicts the effects of a given concentration of a pesticide based on the outcome of already performed experiments using experimental ecosystems. This has the great advantage that the outcome is more realistic. The paper especially discusses how this model can be used to translate measured and predicted concentrations of pesticides into ecological risks, by taking data on measured and predicted concentrations of atrazine as an example. It is argued that this model can be of great use to evaluate the outcome of chemical monitoring programmes (e.g. performed in the light of the Water Framework Directive) and can even be used to evaluate the effects of mixtures.

Keywords: Effect model; Aquatic community; Ecological risk assessment; Pesticides; Case-based reasoning; Atrazine

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1. Introduction

An important topic in the registration of pesticides and the interpretation of monitoring data is the estimation of the consequences of a certain concentration of a pesticide for the ecology of aquatic ecosystems. Solving these problems requires predictions of the expected

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response of the ecosystem to chemical stress. Up until now, a dominant approach to come up with such a prediction is the use of simulation models or safety factors. The disadvantage of the use of safety factors is a crude method that does not provide any insight into the concentration–response relationships at the ecosystem level. For the simulation modelling approach, all available quantitative information on important processes is combined in a mathematical model. However, these models have serious drawbacks, such as: (1) they are often very complex and lack transparency, (2) their implementation is expensive and (3) there may be a compilation of errors, due to uncertainties in parameters and processes.

In this paper, we present an expert model that overcomes these problems. It predicts the effects of a given concentration of a pesticide based on the outcome of already performed experiments using experimental ecosystems. This has the great advantage that the outcome is more realistic. The paper also discusses how this model can be used to translate measured and predicted concentrations into ecological risks, by taking data on measured and predicted concentrations of atrazine as an example.

2. The use of case-based reasoning in risk assessment

Case-based reasoning (CBR) is a problem-solving paradigm that is able to utilise the specific knowledge of previously experienced, concrete problem situations (cases) for solving new problems. CBR is an approach that enables incremental, sustained learning since new experience is retained, making it immediately available for future problems (Aamodt and Plaza, 1994). A very important feature of case-based reasoning is its ability to learn. By adding present experience into the case base, improved predictions can be made in the future.

The Wageningen University and Alterra have developed a case-based reasoning methodology for the prediction of pesticide effects on freshwater ecosystems (Van den Brink et al., 2002a). This methodology is called prediction of the ecological risks of pesticides (PERPEST) and is incorporated into a user-friendly interface (Van Nes and Van den Brink, 2003). It predicts the effects of a certain concentration of a pesticide on various (community) endpoints simultaneously. The database containing the “experiences from the past” was constructed by performing a review of freshwater model ecosystem studies evaluating the effects of insecticides and herbicides. This review was performed to assess the effects on various endpoints (e.g. community metabolism, phytoplankton and macroinvertebrates) and to classify these effects according to their magnitude and duration. This literature review resulted in a database containing the effects of 22 herbicides and 24 insecticides. In total 104 experiments (49 herbicides and 55 insecticides) were evaluated, resulting in 421 cases (208 herbicides and 213 insecticides). A case is a pesticide-concentration combination, so in every experiment on average four concentrations were evaluated. The PERPEST model searches for analogous situations in the database based on relevant environmental fate characteristics of the compound, exposure concentration and type of ecosystem to be evaluated. A prediction is provided by using weighted averages of the effects reported in the most relevant literature references. PERPEST results in a prediction showing the probability of no, slight or clear effects on the various grouped endpoints (see Fig. 1). The ‘no effect’ class is defined as that for which no effects are expected as a result of treatment. The ‘slight effect’ class is assigned when effects are only predicted for individual samplings, especially shortly after treatment. In all other cases, effects are predicted as ‘clear effects’, i.e. a clear response of sensitive endpoints and effects are predicted for subsequent sampling dates. The PERPEST model is described in Van den Brink et al. (2002a) and more technical details can be found in Van Nes and Van den Brink (2003). The model and both documents are available at www.perpest.alterra.nl or www.perpest.wur.nl.

3. Case study with atrazine

3.1. Prediction of effects of atrazine by PERPEST

The PERPEST model was used to predict the effects of atrazine on functional and structural endpoints for a broad concentration range (0.1–10000 μg/L). Cases were weighted on the basis of ‘toxic unit’ (TU), ‘molecule group’ and ‘substance’. This means that cases evaluating the same substance, a substance

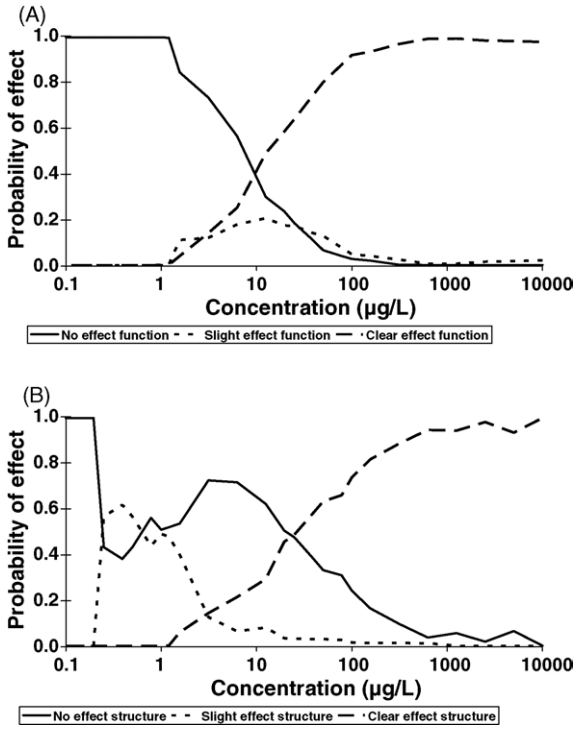

Fig. 1. Relation between the probability of no (connected line), slight (line with small dashes) and clear effects (line with long dashes) on functional (A) and structural (B) endpoints as predicted by the expert model PERPEST for atrazine over a concentration range.

belonging to the same molecule group and/or a similar TU as the TU of the question case to be predicted get a higher weight. Weighing coefficients were optimised using the controlled random search procedure (Van Nes and Van den Brink, 2003). Only cases evaluating TU not differing by more than a factor of 8.3 (a value in the normal range when optimised using controlled random search) from the question case were taken into account. All cases not evaluating photosynthesis inhibiting herbicides were also excluded from the prediction. No distinction was made between exposure regimes, i.e. studies evaluating a single and multiple applications were equally weighed.

PERPEST predicts the effects on eight grouped endpoints of which one represents functional endpoints (community metabolism) and the other seven structural ones. The structural endpoint belonging to the primary producers that showed the largest probability of a clear effect was taken as representative for structural endpoints. In this way graphs showing the probability of no, slight and clear effect on functional and structural endpoints were obtained (Fig. 1).

Fig. 1 shows that clear effects of atrazine start to emerge above 1 μg/L (the actual threshold level is 1.2 μg/L). Slight effects on structural parameters are predicted to occur at very low concentrations of atrazine. This prediction is heavily influenced by the findings of Seguin et al. (2001), who reported slight effects on phytoplankton at a concentration of 2 μg/L. Because a maximum ratio of 8.3 was allowed between toxic units, this experiment influenced the predictions between 0.24 and 16.6 μg/L. This influence was especially large in the lower concentration range (Fig. 1B) because experiments evaluating low concentrations are scarce. Although clear effects on functional endpoints are predicted to occur at lower concentrations compared to structural ones, the probability of clear effects on structural and functional endpoints generally show the same relationship with atrazine concentration. Probability of clear effects starts to emerge at 1.2 μg/L, becoming 50% in the concentration range of 12–25 μg/L and becoming relatively certain at concentrations above 100 μg/L (Fig. 1).

3.2. Linking PERPEST to measured exposure data

Atrazine is principally used for control of certain annual broadleaf and grass weeds, primarily in corn but also in sorghum, sugarcane, and, to a lesser extent, other crops and landscaping. Atrazine is found in many surface and ground waters in North America, and aquatic ecological effects are a possible concern. Applications of atrazine in the Midwestern states of Illinois, Iowa, Nebraska and Indiana accounted for 52% of corn use and 43% of the total atrazine applied in the US in 1993 (Solomon et al., 1996).

Data on the dynamics of atrazine concentrations were downloaded from the website of the National Water Quality Assessment Data Warehouse of the United States Geological Survey. The most extensive data set for a water body from the Midwest states was present for the stream Maple Creek near Nickerson (Nebraska state, Dodge county). On 7 June 2004 only data above the level of detection (0.001 μg/L, measured by GC/MS) were downloaded for this creek. The creek is located in an agricultural area (latitude: 41.6 N and longitude: 96.5 W). Unfortunately, the database does

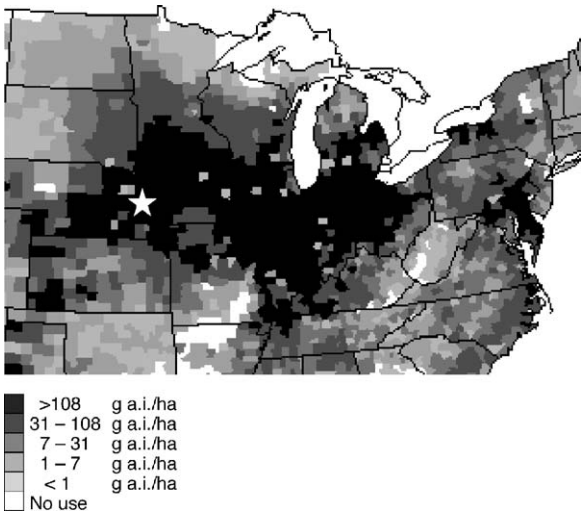

Fig. 2. Estimated annual agricultural atrazine use in 1997 for northeast USA. The star indicates the position of the Maple Creek in Nebraska. Data obtained from the Pesticide National Synthesis Project, which is part of the United States Geological Survey's National Water Quality Assessment Program (NAWQA). Data downloaded from http://ca.water.usgs.gov/pnsp.

not provide any more information on crops grown near this creek, but it is situated in an area with high atrazine use (Fig. 2). The data run from 30 April 1997 to 16 September 2003 and consisted of 124 values.

Fig. 3 shows the dynamics of atrazine in the Maple Creek together with the threshold for clear effects (1.2 μg/L) as calculated by PERPEST. Concentrations

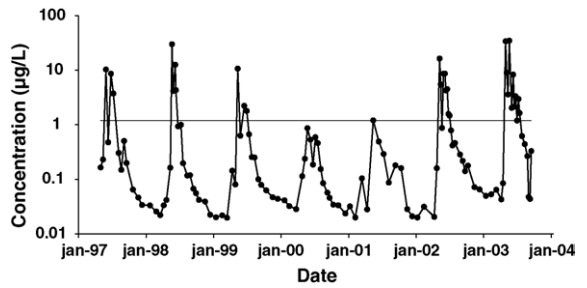

Fig. 3. Dynamics of atrazine concentration in the Maple Creek near Nicker son (Nebraska state, Dodge county). Data obtained from the National Water Quality Assessment Data Warehouse of the United States Geological Survey (assessed via http://water.usgs.gov/nawqa/data). The geometric mean concentration is 0.27 μg/L, the maximum 34.8 μg/L). The thin line denotes the threshold level for clear effects as calculated by the PERPEST model.

exceeding this threshold were all measured between 30 April and 15 July and no exceedence was measured in the years 2000 and 2001. Highest concentrations were measured in 2003 (34.8 μg/L) followed by 1998 (30.0 μg/L), 2002 (16.4 μg/L), 1999 (10.7 μg/L) and 1997 (10.3 μg/L). The geometric mean concentration is 0.27 μg/L; the maximum concentration of 34.8 μg/L was measured on 20 May 2003.

Fig. 4 shows the probabilities of no, slight and clear effects as predicted by PERPEST for the maximum concentration (Fig. 4A) and geometric mean concentration (Fig. 4B). These concentrations were chosen as examples, for estimating the effects of atrazine it might be more relevant to chose another mean concentration, e.g. the geometric mean concentration of the worst-case time window for each month or week. It is clear that the maximum concentration poses a serious risk to the functioning and structure of aquatic ecosystems. For community metabolism, maximum probabilities of clear effects were calculated to be larger than 50% for macrocrustaceans and insects and phytoplankton, while maximum probabilities of between 25 and 50% were calculated for fish and tadpoles, macrophytes and periphyton. A small or zero chance of a clear effect were only indicated for zooplankton and molluscs. A zero probability of a clear effect is calculated for all endpoints for the mean concentration, although data for fish and tadpoles, macrocrustaceans and insects and molluscs were missing. These groups, however, are not expected to be the most sensitive to atrazine (Maltby et al., 2005). Data on primary producers are available in this concentration range, though sparse (between 1 and 4 cases for each grouped endpoint).

Fig. 5 shows the predicted probability of clear effects on the most sensitive endpoint related to functioning (A) and structure (B) of aquatic ecosystems for the dates at which the concentrations exceeded the threshold values of 1.2 μg/L. The error bars show the 95% confidence intervals, as calculated by an internal bootstrapping method (Van Nes and Van den Brink, 2003). The highest probabilities for effects on the functioning and structure of aquatic ecosystems are calculated for the year 2003. In 43% of the cases there is a chance of 25% or greater that a clear effect will occur on a functional parameter; in 14% of the cases this chance is 50% or more. These probabilities are comparable for structural parameters (43 and 11%, respectively). If

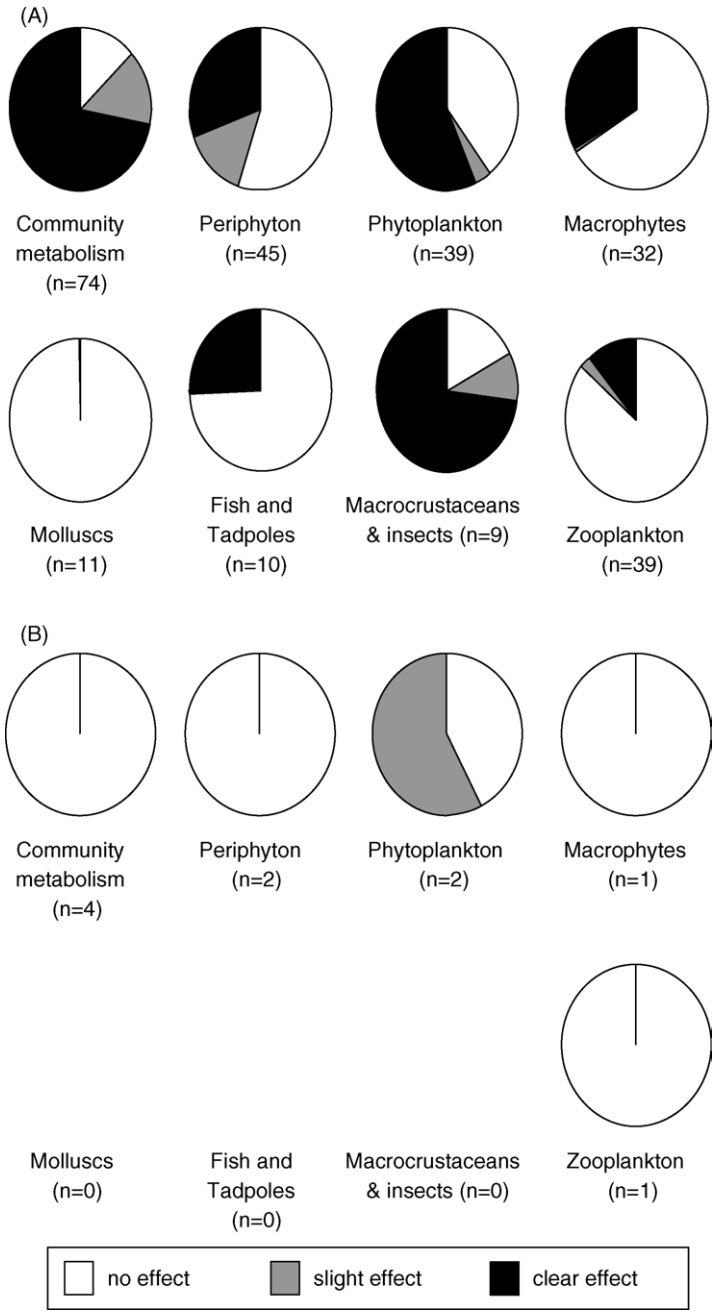

Fig. 4. Effects as predicted by PERPEST of 34.8 μg/L (A) and 0.27 (B) μg/L atrazine on eight grouped endpoints.

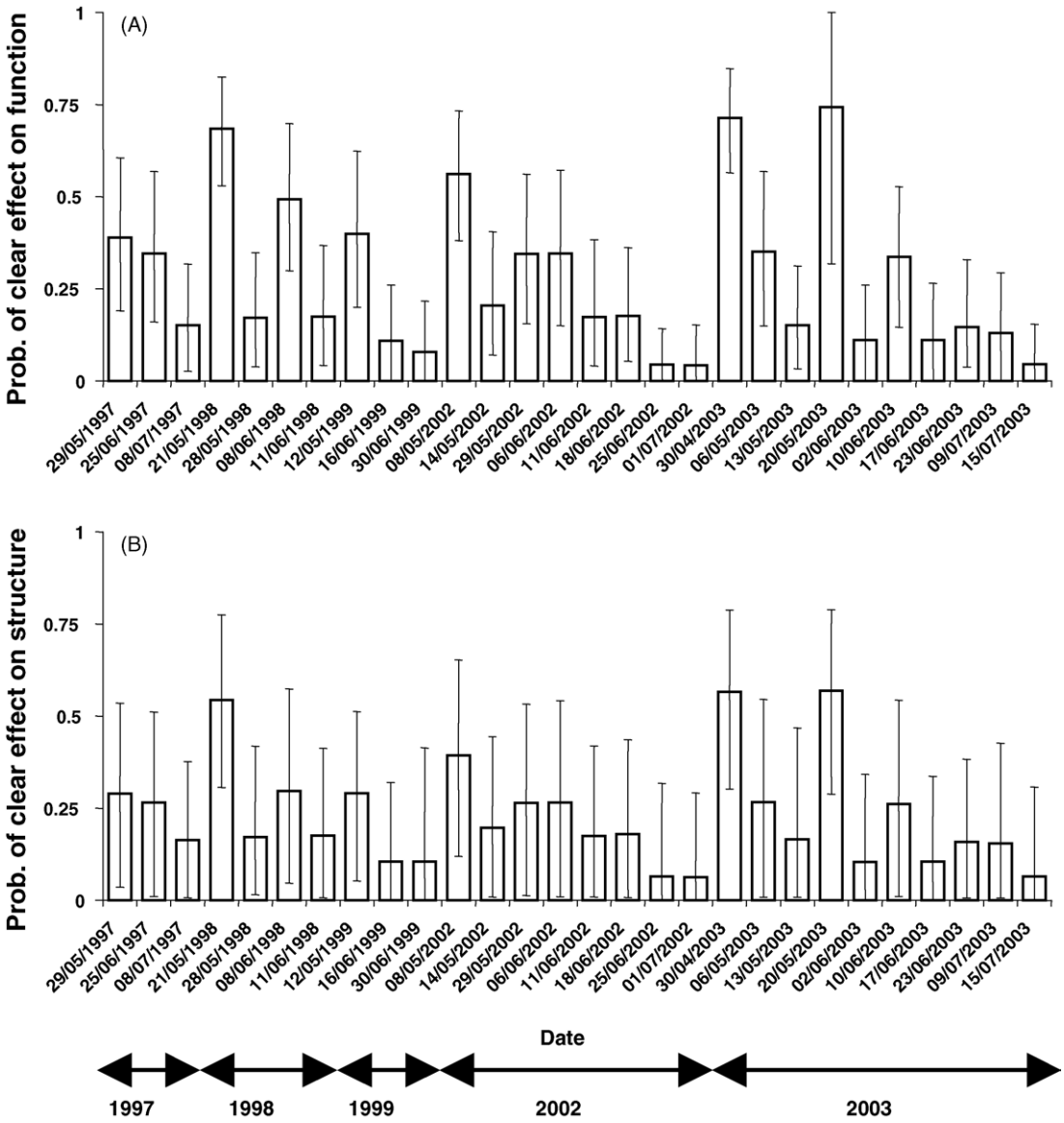

Fig. 5. Calculated probabilities (plus 95% confidence interval) of clear effects for the concentrations exceeding the threshold levels in Fig. 1. (A) Denotes the probability of a clear effect on functional parameters, whereas (B) shows the probability of clear effects on structural parameters belonging to the primary producers.

the structure and functioning of the model-ecosystems as well as the exposure regime used in the experiments incorporated in PERPEST are representative for Maple Creek, it is very likely that atrazine contamination affected the aquatic community during the last 7 years, in particular in the year 2003.

3.3. Linking PERPEST to predicted exposure data

Modelling was undertaken to predict variability in concentrations of atrazine in a field-side ditch arising from transport in sub-surface drainflow. The preferential flow model MACRO Version 4.3 (Jarvis, 1994) was

used to simulate transport in drainflow and output was fed into a simple mixing model to calculate concentrations in the ditch on a daily basis. MACRO divides the soil pore system into the soil matrix where flow is relatively slow and driven by convection and dispersion (micropore domain) and a region with preferential flow pathways, which deliver water and solutes rapidly to depth (macropore domain). The main application of MACRO is to simulate flow through structured soils where rapid movement of water and solutes through cracks, fissures or biopores is important. MACRO has been evaluated against a number of datasets on leaching of pesticides or non-interactive solutes (Bergström, 1996; Brown et al., 1998; Larsson and Jarvis, 1999). Although discrepancies from measured data are occasionally observed, results indicate that MACRO is able to describe the main patterns of solute transport resulting from preferential flow.

The simulated scenario comprised a 1 ha clay loam field (topsoil 32% sand, 42% silt, 26% clay and 2.3% organic carbon) cropped with maize and treated with atrazine (1.5 kg/ha) in the spring of 30 successive seasons. Drainflow fed into a ditch 100 m in length, 1 m in width and 0.3 m in depth. Temporal variability in transport in drainflow was considered by using a 30-year run of daily weather data (annual rainfall 403–830 mm, average 602 mm; mean annual minimum and maximum air temperature 5.4 and 13.2 °C, respectively). Variability in predicted drainflow volumes and concentrations in the ditch arising from parameter uncertainty was estimated using Monte Carlo simulations based on Latin Hypercube sampling from distributions of model input parameters.

Results from a model sensitivity analysis for MACRO (Dubus and Brown, 2002) guided the selection of variables for probabilistic modelling. The authors investigated the sensitivity of input parameters for MACRO for transport of two pesticides through a sandy loam and a clay loam soil. Results for the clay loam soil were used here and showed pesticide leaching to be most sensitive to parameters describing the sorption and degradation of the pesticide and to hydraulic parameters comprising TPORV (total porosity), ZN (macropore tortuosity), XMPOR (boundary water content), KSM (boundary hydraulic conductivity) and ASCALE (aggregate half-width).

Probability density functions representing the variability of pesticide and soil properties were assigned on the basis of experimental information (pesticide properties) or expert judgement (soil parameters). Details are provided in Table 1. A total of 500 sets of input parameters was randomly generated from the distributions and used as the basis for simulations. Parameters were considered to be independent of each other for the sampling. A total of 95 input files out of 500 were rejected by MACRO due to randomly sampled values for the boundary water content (XMPOR) being larger than those for the total porosity (TPORV).

Predicted atrazine concentrations in the receiving ditch were calculated assuming that the residence time of water in the ditch was 1 day. Thus, the daily input of drainflow and pesticide always entered the same volume of uncontaminated water. We are aware that choosing smaller time-steps (e.g. hour) would yield different results, i.e. higher peak concentrations. Atrazine is not killing primary producers within such small timescales but inhibits photosynthesis. The latter inhibition will be translated into effects only when exposure is prolonged (days or weeks). For the sake of the example, we chose for daily averages for convenience.

Annual drainflow ranged between 126 and 405 mm, whereas annual average drainflow for the 405 simulations ranged between 250 and 302 mm. The maximum concentration of atrazine in the ditch in each year

Table 1
Summary of distribution statistics for the seven primary parameters varied within Monte Carlo modelling

Parameter	Description	Distribution	Mean	Variance
ASCALE	Effective diffusion pathlength (mm)	Log-normal	10.0	9.39
DEG	Degradation rates (d^{-1})	Log-normal	2.12×10^{-2}	1.07×10^{-4}
KSM	Boundary hydraulic conductivity ($mm\,h^{-1}$)	Normal	1.32×10^{-1}	7.83×10^{-4}
TPORV	Saturated soil water content (vol%)	Normal	51.9	5.28
XMPOR	Boundary soil water content (vol%)	Normal	44.1	3.65
ZKD	Sorption coefficient ($cm^3\,g^{-1}$)	Log-normal	3.68	4.31
ZN	Pore size distribution factor (macropores)	Normal	3.49	1.01×10^{-1}

simulated ranged between 0 and 87 μg/L, whereas the average of the 30 maxima in each simulation ranged between 0.1 and 42 μg/L. The maximum daily concentration of atrazine in the ditch was extracted for each of 30 years in each of the 405 successful simulations. The resulting 12,150 values were ranked into the cumulative frequency distribution shown in Fig. 6.

The probabilistic distributions for exposure and effects (Figs. 1 and 6) can be combined to assess the likelihood of effects occurring. This has often been achieved using a Joint Probability Curve (JPC, ECOFRAM, 1999; Aldenberg et al., 2002), which is an exceedence curve showing the joint probabilities of exceeding a concentration and associated probabilities of clear effects. The JPC for these data sets is shown in Fig. 7, in which the mean and the confidence intervals (obtained by internal bootstrapping, Van Nes and Van den Brink, 2003) show the influence of, respectively, variability and uncertainty in the assessment of effects. The influence of variability and uncertainty is combined for the exposure calculation. It would be possible to separate the influence of variability in weather patterns from that of the combined variability and uncertainty in the most sensitive model parameters.

The curves can be read as follows (examples are clarified by dotted lines in Fig. 7A):

- The 90th percentile exposure concentration (= 0.1 frequency on *y*-axis) is estimated to result in clear effects on community metabolism with a frequency of 49% (95% confidence interval 31–69%), assuming that the exposure model is correct and that mesocosm studies directly represent effects in the field.

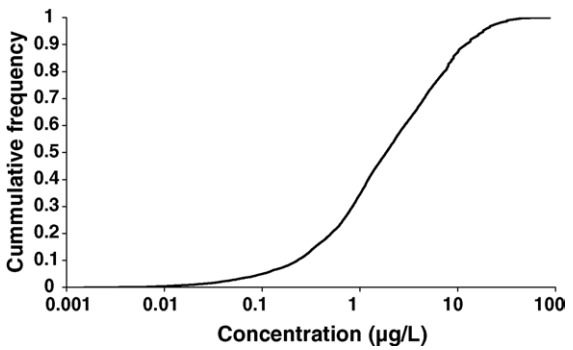

Fig. 6. Cumulative distribution of atrazine exposure predicted for the ditches as a result of sub-surface drainflow scenario.

- A 25% frequency of clear effects on community metabolism occurs for 77th percentile (95% confidence interval 56–86%) of the exposure distribution assuming that the exposure model is correct and that mesocosm studies directly represent effects in the field.

In the current instance, both axes of Fig. 7 can be interpreted as proportions of application events, so they can be combined to estimate the overall frequency that clear effects would result (Solomon et al., 2002). This overall frequency that clear effects will occur is equal to the area under the curves of Fig. 7.

The chart showing the overall frequency (Fig. 8) shows that:

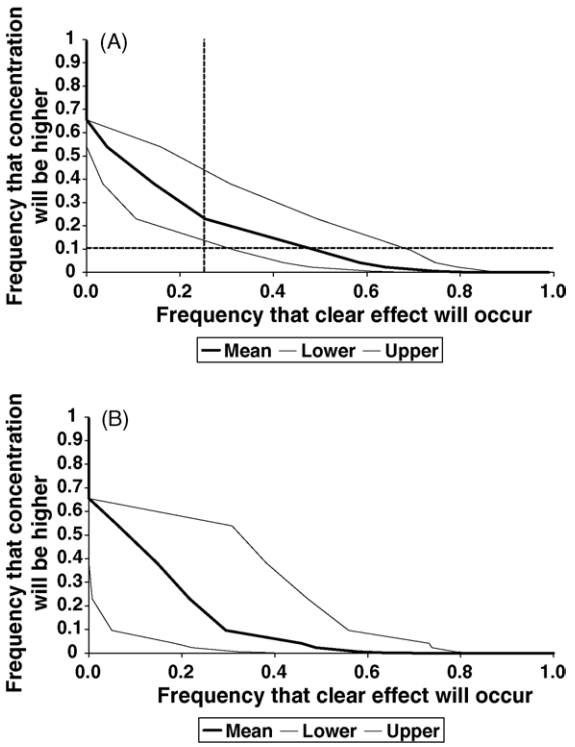

Fig. 7. Joint curve showing the predicted frequency of exceeding a given initial exposure concentration in predicted ditches and the frequency that the concentration would result in clear effects on community metabolism (A) and structural endpoints (B) in a mesocosm study (thick line = mean prediction; thin lines = 95% confidence interval). Line in (A) refer to a numerical example of interpretation described in the text.

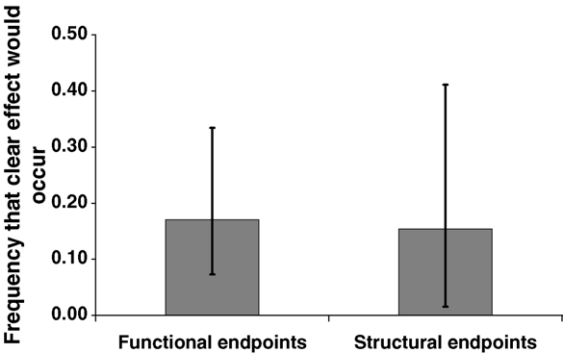

Fig. 8. Overall frequency that exposure of the predicted ditches would result in clear effects on community metabolism and structural parameters in a mesocosm study. Line shows 95% confidence interval.

- The estimated frequency of clear effects on community metabolism is 17% (95% confidence interval 7–33%) assuming that the exposure model is correct and that mesocosm studies directly represent effects in the field.
- The estimated frequency of clear effects on structural parameters is 15% (95% confidence interval 2–41%) assuming that the exposure model is correct and that mesocosm studies directly represent effects in the field.

4. Discussion

A key advantage of PERPEST over single species/safety factor analyses is that it decreases the uncertainty of extrapolating to the ecosystem level. As the effects data are based on mesocosm studies there is still the uncertainty of extrapolating the mesocosm data to the field. The benefit of PERPEST is not only that it removes some uncertainty by included experience from other pesticides but that it quantifies the uncertainty by taking a probabilistic approach and provides uncertainty limits to predicted values. A very popular method to extrapolate from the species to the community level is the species sensitivity distribution (SSD) concept. In this concept a statistical distribution is estimated from a sample of toxicity data (i.e. L(E)C50 or NOEC values) and visualised as a cumulative distribution function (Posthuma et al., 2002). Species sensitivity distributions are used to calculate the concentrations at which a specified proportion of species will be affected, referred to as the HCp, the hazardous concentration for p% of species. Often the HC5 is used as a threshold value safe for the aquatic ecosystem (Maltby et al., 2005). Although there is growing empirical evidence that the HC5 (or the lower 95% limit thereof) are indeed protective for the aquatic ecosystem (Versteeg et al., 1999; Van den Brink et al., 2002b; Schroer et al., 2004; Maltby et al., 2005; Hose and Van den Brink, 2004; Brock et al., 2004), the use of the approach implies a significant number of assumptions. A few of these assumptions are (Versteeg et al., 1999; Forbes and Calow, 2002):

1. The sample of the species on which the SSD is based is a random selection of the community of concern, and is representative for this community.
2. Interactions among species do not influence the sensitivity distribution.
3. Since functional endpoints are normally not incorporated into the SSD, community structure is the target of concern.
4. The laboratory sensitivity of a species approximates its field sensitivity.
5. The endpoints measured in the toxicity tests on which the SSD is based are ecologically relevant.
6. Since in SSD all species have equal weight, it is assumed that all species are equally important for the structure and functioning of the ecosystem of concern.
7. The real distribution of the sensitivity of the community is well modelled by the selected statistical distribution.
8. The number of species data used to fit the distribution is adequate from a statistical, ecological and animal welfare point of view, to describe the real distribution of the sensitivity of the community.
9. The protection of the prescribed percentile of species ensures an ‘appropriate’ protection of field ecosystems.

As a result of these assumptions, the use of the SSD concept is also criticised (Forbes and Calow, 2002). Since PERPEST is based on results from ecosystem level experiments, most of the assumptions made when applying the SSD approach are not made when using PERPEST. However, when PERPEST is applied for a

particular case (e.g. the Maple Creek) some assumptions are made:

1. The cases upon which the prediction are made are representative for the question case with respect to ecosystem structure and functioning and exposure regime.
2. The calculations of dissimilarity and transformation, standardisation and weighing of variables used in PERPEST are adequate for making predictions.
3. The number of cases present in PERPEST is sufficient for making a prediction.

The major sources of variation left are the variability of responses between different ecosystem types and the question of how representative the structure and functioning of the model-ecosystems and exposure regime used in the experiments incorporated in PERPEST are for the question case. It has been argued by some authors that threshold values and direct effects observed for the same compound were very similar in different aquatic ecosystems. Different studies conducted with the same insecticide (e.g. chlorpyrifos, esfenvalerate and lambda-cyhalothrin) yielded similar critical threshold values and effects for different types of ecosystems ranging from streams to ponds (Brock et al., 2000a; Van Wijngaarden et al., 2005). A literature review for photosynthesis-inhibiting herbicides described in Brock et al. (2000b) showed that effects, when expressed as toxic units, start to emerge at similar threshold values in different types of ecosystems. This variability in response is, together with the variability in exposure regimes, incorporated into the confidence limits of the predicted probability, and is thus explicitly expressed in the output of PERPEST. Limiting the prediction to studies only involving a single or a multiple application reduced the uncertainty of the prediction on the one hand because the exposure regime is more uniform between the cases but increases the uncertainty on the other side because the prediction is based on less observations.

On the exposure side, there is a chance that PERPEST might underestimate the real probabilities of clear effects for measured concentrations as water samples might not have been taken at times where atrazine concentrations are largest in the creek. This is not a shortcoming of PERPEST as such, but a methodological problem of chemical monitoring in general. In the case of modelled exposure, PERPEST encompasses chronic effects without the need to manipulate exposure concentrations in some artificial way (e.g. time weighted average concentrations) because one can simply use the modelled instantaneous concentration and compare it to the dosing concentration used in the experimental data included in PERPEST. This approach relies on the assumption that dissipation of pesticides in the mesocosm experiments is similar to that in the creek (or at least that the former occurs more slowly, thus giving a conservative assessment).

Until now, only SSD curves have been used to define the effect side of JPCs. The JPC exceedence profile was recommended by the Aquatic Working Group of ECOFRAM (ECOFRAM, 1999) and offers a useful tool for communicating risks as it allows what-if questions to be addressed and gives the risk assessor a method for assessing the effects of changes in assumptions, such as the choices of different percentiles from the concentration distributions or choices of different percentiles for accepted probabilities of effects (Solomon and Takacs, 2002). The main difference from analyses based on a SSD is that the use of PERPEST entails the acceptance of the fact that a probability that a clear effect will occur given a certain percentile rather than the acceptance of a percentile for the proportion of total species at risk. For instance, the JPC for structural endpoints indicated that the 90th percentile of the predicted atrazine exposure has a 30% probability of causing a clear effect. Choosing a 80th or 95th percentile will change the predicted probability substantially (Fig. 7). In this way the consequences of changing the objectives for the risk assessment are made explicit. To overcome the tedious interpretation of JPC and the management choices associated with it, we also calculated the overall risk (Fig. 8). Though less informative, it may provide an easier way to communicate risks with risk managers and people involved in pesticide registration. When using the overall risk, only a single threshold for an acceptable risk has to be defined.

In the current example, ‘clear effects’ are defined quite broadly, as a clear response of one or more of the sensitive endpoints and effects being predicted for subsequent sampling dates. This definition may range from one species showing clearly reduced numbers for a month to a complete extermination of groups of species for several months. To be able to differentiate between short-term and long-term effects, PERPEST also offers

the possibility to refine the 'clear effects' class in three categories: clear short-term effects with recovery within 8 weeks, short-term effects with unknown recovery (the cases on which the prediction is based upon had an experimental period shorter than 8 weeks) and clear long-term effects with recovery taking longer than 8 weeks. This refinement was not included in this example for simplicity, but might be of great importance for setting threshold values for acceptable probabilities of clear effects. Potential for recovery is increasingly important for regulatory decisions concerning pesticides in Europe (Giddings et al., 2002).

The approach described in this paper also has some obvious drawbacks: (1) often only very few really comparable cases are available and (2) specific cases are often too easily generalised. This led us to the idea that it would be good to seek the best of both worlds by using case-based reasoning as a mimic of the experts' approach and subsequently fine-tuning the results with the aid of simple ecological models. Branting et al. (1997) called this integration of case-based reasoning and model-based reasoning 'model-based adaptation' and described an example involving a system for rangeland grasshopper management. The latter part of this approach is new in the field of predictive modelling of effects and will yield an approach that better estimates the effects of chemical stress and management on the ecology of aquatic ecosystems and also a modelling concept that can be used to tackle a variety of problems. In the light of the tiered approach that has been adopted in risk assessment and the availability of models, this integration looks promising for the field of ecological risk assessment of pesticides for their registration on the European market.

Chemical monitoring is often performed to evaluate the quality of surface waters for regulatory purposes and/or to evaluate environmental status and trends. Such monitoring activities are expected to increase in Europe due to the Water Framework Directive, as adopted on 23 October 2000 to establish a framework for the Community action in the field of water policy (EU, 2000). For surface waters, this framework defines good ecological and chemical status, which needs to be monitored in time. In this paper, we showed an example of how these monitoring data can be translated into ecological risks. It is often mixtures of pesticides rather than single compounds, which are found to be present in surface waters. It would therefore be a great improvement if PERPEST could estimate the overall ecological risks associated with measured concentrations of different pesticides. This can be done with PERPEST by adding the peak concentrations of chemicals with a similar mode of action as toxic units (concentration addition; Deneer, 2000). By adding a hypothetical pesticide representative for a certain mode of action to the list already present in PERPEST, the risk can be obtained for all compounds which share the same mode of action and which have been included in the monitoring exercise. The individual risks can be added up to an overall risk using the concept of response addition (Deneer, 2000). In addition, the combined risk assessment of nutrients and pesticides would enable an overall risk assessment of farm practices. This could be done by adding experiments performed with nutrients to the database, although little is known about the combined action of nutrients and pesticides.

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