Taking uncertainty into account in pesticide fate modelling

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Current environmental risk assessment procedures for pesticide registration in the EU rely on the comparison between exposure and ecotoxicological endpoints (surface waters) or a legal threshold concentration (groundwater). A tiered approach is implemented to concentrate on those compounds which might be harmful to the environment and not penalise those which pose little environmental threat. Relevant ecotoxicological endpoints are typically derived by laboratory tests using a range of representative organisms although predictive models such as QSARs (Quantitative Structure Activity Relationships) are sometimes used in the early stages of the risk assessment. In contrast to the derivation of effect concentrations, the estimation of Predicted Environmental Concentrations for exposure (PEC's) relies heavily on the use of predictive environmental fate models, especially at higher tiers.

Deterministic models which are most commonly used to estimate PEC's for groundwater are PELMO, PRZM, PEARL and MACRO. A detailed presentation of the capabilities of the different models can be found elsewhere (FOCUS, 2000). The estimation of the fate of crop protection products in surface waters is less harmonised at present and a range of approaches are used to estimate PEC's, from simple dilution calculations through the use of reference data (e.g. Ganzelmeier tables for spray drift) to deterministic models such as the Dutch model TOXSWA. Inputs to a surface water body via soil erosion, run-off or drainage can be estimated using those leaching models which integrate a description of relevant processes.

For surface waters, the ratio between PEC and ecotoxicological endpoints is calculated (termed TER for Toxicity:Exposure Ratio) and compared to threshold values which are dependent on the organism considered (typically 10 or 100). A compound is considered to pose little threat to surface water organisms if the TER exceeds the thresholds. These trigger values can be considered as safety factors which account in part for the uncertainty in the TER itself. For groundwater, PEC's are compared to a threshold concentration of 0.1 µg a.i./l, irrespective of the toxicity and ecotoxicity of the compound.

A schematic representation of the current pesticide registration procedures for assessing the risk posed by the product to the environment is provided in Figure 1.

## Sources of uncertainty in pesticide fate modelling

Uncertainty in the modelling of pesticide fate in the environment originates from a variety of sources. Uncertainty may result from model inadequacy (the inability of the model to simulate reality even if the models has the right input), from variability and uncertainty in the values for input parameters or from the influence of the modeller.

Most variables measured on samples taken in the field are variable in space and in time. These

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Figure 1 – Schematic representation of current environmental risk assessment procedures.
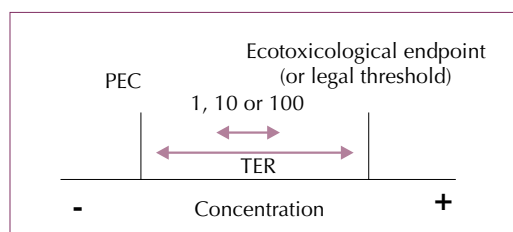
include for instance soil properties (e.g. particle size distribution, organic matter content, bulk density, soil hydraulic properties) and sorption and degradation characteristics of a compound. Wood *et al.* (1987) reported Koc values varying from 66 to 1445 l/kg in a 4-ha field (Coefficient of Variations 17-47%) while Elabd *et al.* (1986) reported a CV of 38% for the Koc of napropamide in a 0.6-ha plot. Walker *et al.* (2001) found large variation of isoproturon degradation in 30 samples taken from a 5-ha field (DT50 6.5 to 30 days). Apart from natural variations at the field scale, variability may arise from the use of different sampling techniques in the field, differences in sample storage and preparation (e.g. frozen vs. refrigerated samples; air dried vs. moist samples), the use of different procedures for analytical measurements or different environmental conditions in the laboratory.

Significant uncertainty is expected to originate from the parameterisation of the model. The attribution of values to input parameters may be based on the use of data collected in the field or in the laboratory, on general relationships established by research groups (e.g. pedo-transfer functions, QSARs) or on expert judgement (an educated decision based on the experience of the individual). The derivation of DT50 values to be used in the modelling from laboratory degradation data is an important step in the

parameterisation. Leake *et al.* (1995) used a degradation dataset (decrease in pesticide concentrations over time) and calculated DT50 values using a range of equations and fitting packages. Resulting DT50 values ranged between 4 and 93 days (mean 27.9 days; median 21.0 days). In a recent evaluation exercise (Vanclooster *et al.*, 2000), a significant variability in model predictions was obtained between different modellers although they all used the same basic information to undertake model parameterisation.

Uncertainty might also be introduced once the model has been run since model output is often manipulated (e.g. for comparison with experimental data). Finally, decision-making based on an identical set of model results might be subject to uncertainty. A number of sources of uncertainties on the predictions of pesticide concentrations in an environmental media are rarely acknowledged in the literature. These include the influence of the selection of a specific model or the inadequate use of models. All the different sources of uncertainty will aggregate as the modelling progresses (Figure 2).

Although sources of uncertainty are clearly numerous and may affect model predictions which are later used in the decision making with regard to the placement of crop protection products on the market, uncertainty is not taken into account in the modelling carried out for pesticide registration. Integrating uncertainty in modelling can be achieved through a number of techniques, the most versatile being the Monte Carlo approach.

Taking uncertainty into account in the modelling

The traditional approach to pesticide fate modelling is to assign values to each model input parameter and to run the model once. In contrast, the Monte Carlo approach is based on numerous runs of the model. A probability density function is attributed to each input parameter to be included in the analysis. This reflects the fact that these parameters are considered uncertain and can take a range of values. A large number of input values for each parameter (say, 1000 values) are sampled randomly from the probability density functions and these are used to generate 1000 model input files. The model is run for all these input files and model outputs are aggregated to enable a presentation of the results

Figure 2 – The increase in the overall uncertainty as modelling progresses.
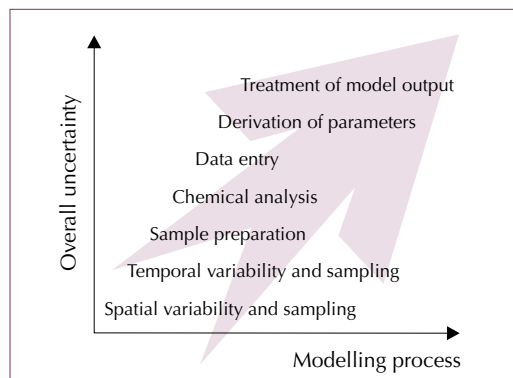
in probabilistic terms. The whole Monte Carlo approach is often referred to as "probabilistic modelling". The following sections explain technical procedures in more detail.

Selection of parameters

Although including all model parameters in a Monte Carlo analysis is technically possible, it is not desirable because this would involve a large number of model runs and attributing adequate probability density functions to each parameter would prove difficult. Parameters which need including in the analysis are those which are uncertain and which significantly influence model predictions. This latter point is traditionally addressed by performing a sensitivity analysis for the model. Although performing such an analysis for the situation at hand is desirable, literature information can also be used. Dubus *et al.* (2000) performed sensitivity analyses for the four pesticide leaching models which are used for pesticide registration in Europe and identified for each model those parameters which most influence predictions for groundwater recharge and pesticide leaching. They found that in most model-scenario combinations considered, models were most sensitive to parameters related to sorption and degradation. An example of results for the MACRO model is provided in Figure 3, in which input parameters have been ranked by decreasing influence on model predictions. More details including the key to parameter names can be found in Dubus & Brown (2002).

Attribution of probability distribution functions

The attribution of probability density functions is a difficult task which is key to the whole probabilistic approach. Probability density functions which are traditionally assigned to input parameters of pesticide leaching models are the normal, log-normal, uniform or triangular probability distributions. Distribution fitting on the basis of statistical tests can be used where data on the variability of parameter values are available. If there are no or few data, literature information on the expected variation or expert judgement may be used.

Sampling and model runs

Monte Carlo sampling into the assigned probability density functions is carried out to generate
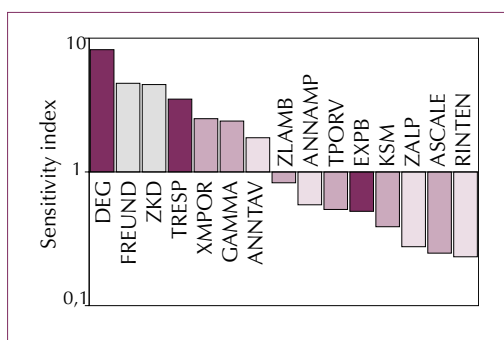
◀ Figure 3 – Example of sensitivity analysis results for the MACRO model.

values for input parameters. The traditional Monte Carlo approach to sampling requires a large number of samples to cover the parameter space. The stratified sampling technique known as Latin Hypercube Sampling (LHS) is an efficient sampling alternative which allows the reduction of the number of runs. The replacement of parameter values in input files, the running of the model and the extraction of selected model output can be easily automated using packages such as SENSAN (Doherty, 2000).

Examination of results

Model predictions for each run are ranked and displayed in a cumulative distribution function (CDF). An example is provided in Figure 4. The chart can be used to estimate the probability of simulating a concentration above or below a particular concentration. In Figure 4, concentrations below 0.07 µg/l are predicted in 75% of the cases and the probability of the pesticide concentration exceeding the threshold of 0.1 µg/l is *ca.* 15%.

Conclusions

Conducting probabilistic modelling using Monte Carlo is relatively simple and the approach can be transferred to any field of science where
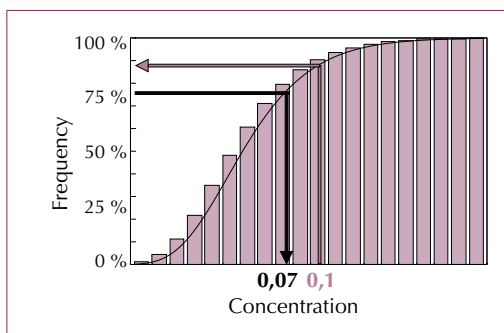
◀ Figure 4 – Example of probabilistic modelling results.

models are used. Distributions of exposure concentrations generated by probabilistic modelling using pesticide leaching models can be compared to threshold concentrations (e.g.

an ecotoxicological endpoint) or to a species sensitivity distribution when the information is available (Figure 5). Taking uncertainty into account provides a more realistic and transparent assessment of the risk of environmental impact compared to the TER approach currently implemented in pesticide registration. Decision makers have the opportunity to look at the wide range of possible outcomes without the limitations of the point estimate methods. The main limitation of the probabilistic approach is that it only considers the uncertainty associated with the model input parameters. Other types of uncertainty, such as the inability of a model to fully represent field data, are ignored.   ❑
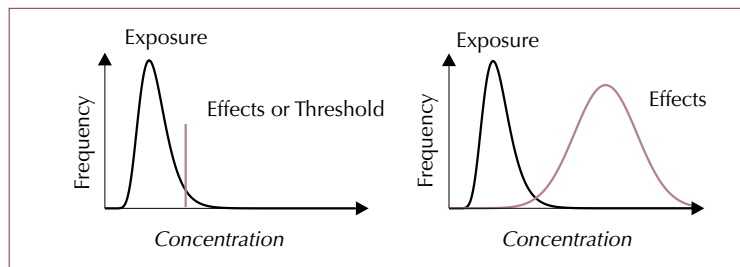
▲ Figure 5 – Revised risk assessments on the basis of probabilistic modelling.

Abstract

Pesticide fate models play an important role in risk assessment procedures for registration of crop protection products both in Europe and in the US. Although sources of uncertainty in pesticide fate modelling are numerous, uncertainty is not explicitly taken into account within current procedures for registration modelling. The paper briefly reviews the main sources of variability leading to uncertainty in model input parameters and present a Monte Carlo framework for taking uncertainty into account in the modelling. The approach is more realistic and transparent than the traditional risk quotient approach and is likely to benefit all stakeholders, from the public through the industry to the regulators.

Résumé

Les modèles de transfert de solutés dans les sols sont largement utilisés dans l'estimation du risque environnemental pour les produits de protection des plantes aussi bien dans le contexte européen qu'américain. Bien que les sources d'incertitude liées à cette modélisation soient nombreuses, l'incertitude n'est pas prise en compte explicitement dans l'approche des Ratios Toxicité/Exposition. Cette communication présente les principales sources d'incertitude dans la paramétrisation des modèles de transfert et explique les fondements de l'approche Monte Carlo appliquée à l'estimation du transfert de pesticides vers les eaux souterraines. L'intégration des incertitudes dans la modélisation permet une évaluation du risque plus réaliste et plus transparente. L'adoption de ces méthodes dans l'homologation des pesticides en Europe paraît désirable.

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Other references and informations : http://www.cranfield.ac.uk/echochemistry