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Uncertainty analysis of USES 3.0
Improving risk management through probabilistic risk assessment of agricultural pesticides

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Abstract

Risk assessment of pesticides in the Netherlands is carried out using the computerised Uniform System for the Evaluation of Substances (USES). In USES the measure of risk is a single-point or deterministic estimate. Here, it is shown how a probabilistic assessment, incorporating knowledge about uncertainty and variability, can provide the decision-maker with improved insights into the risk management of pesticides. Advantages and possibilities of a probabilistic assessment are presented and provided with examples of calculations. This document is only intended for discussion; further efforts will be needed before a quantitative uncertainty analysis can be incorporated into the routine assessment of pesticides.

Preface

The USES model is developed to perform a quick, consistent and transparent risk assessment of among others pesticides. An up-to-date scientific basis is necessary to find an answer for the increasingly complex policy questions concerning the risk assessment of pesticides. The uncertainty analysis for the assessment of pesticides with USES serves this purpose. The Dutch Directorate-General for the Environment commissioned the National Institute of Public Health and the Environment (RIVM) to carry out this project. This report is written for decision-makers working in the framework of legislation of pesticides and demonstrates how probabilistic risk assessment may improve risk management.

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Samenvatting

De risicobeoordeling van bestrijdingsmiddelen in Nederland volgt de EU procedure volgens richtlijn 91/414/EEC. In Nederland wordt de risicobeoordeling uitgevoerd met het computermodel Uniform Systeem voor de Evaluatie van Stoffen (USES). USES gebruikt een deterministische schatting of puntschatting, die wordt beschreven door het quotiënt van de voorspelde milieuconcentraties en een niet geëxtrapoleerde toxiciteitswaarde voor de beschouwde organismen. Een deterministische benadering kan bruikbaar zijn voor een eerste schatting, maar deze methode houdt geen rekening met de reeks van mogelijke resultaten en het feit dat sommige resultaten vaker voorkomen dan andere. Beleidsmakers kunnen worden misleid door een deterministische benadering, omdat puntschattingen ten onrechte als nauwkeurig kunnen worden beschouwd. Een onzekerheidsanalyse kan waardevol zijn voor beleidsmakers, omdat rekening wordt gehouden met de variatie, door middel van het toekennen van een probabilistische verdeling aan de invoerwaarden, wat leidt tot een probabilistische verdeling van de risico's. Met een probabilistische aanpak zijn de volledige reeks van het resulterende risico en de belangrijkste bronnen van onzekerheid beschikbaar. Zo'n aanpak laat de informatie zien die nodig is om de risicobeoordeling te verfijnen.

In dit rapport worden voorbeeldberekeningen gepresenteerd om de beleidsmaker te voorzien van aanvullende inzichten betreffende probabilistische risicobeoordelingen voor pesticiden. Ook wordt behandeld hoe een probabilistische risicobeoordeling kan worden geïnterpreteerd. De voorbeeldberekeningen laten zien dat beleidsmakers van meer informatie worden voorzien waarop ze hun beslissingen kunnen baseren. In deze voorbeelden worden alleen stofspecifieke onzekerheden gekwantificeerd en zijn andere bronnen van onzekerheid en variabiliteit niet meegenomen. Een onzekerheidsanalyse kan direct invloed hebben op de toelating van bestrijdingsmiddelen. In het Handboek voor de Toelating van Bestrijdingsmiddelen (HTB) staan achtergrondgegevens over de overschrijdingsfactoren van de normen voor waterorganismen en de uitspoeling naar het grondwater (CTB, 1999). Voor deze eindpunten is een extra onzekerheid van 100 opgenomen in het HTB. Deze factor kan misschien worden verlaagd als een onzekerheidsanalyse wordt toegepast. De onzekerheden in de resultaten van USES zijn afhankelijk van de stofeigenschappen. Over het algemeen is de degradatie de belangrijkste bron van onzekerheid. Voor enkele bestrijdingsmiddelen zijn voor de risico's voor waterorganismen ook Kom, dampdruk en oplosbaarheid belangrijk. Voor de uitspoeling naar grondwater is niet alleen degradatie, maar ook Kom een belangrijke bron van onzekerheid. De onzekerheid van het resultaat wordt minder gevoelig voor degradatie als de onzekerheid van de toxiciteitswaarden wordt meegenomen. Verder wordt in dit rapport nog een mogelijkheid gepresenteerd om op een nauwkeurige manier de onzekerheidsanalyse in de effectbeoordeling mee te nemen.

Dit rapport moet worden gezien als een discussiedocument voor beleidsmakers, om vertrouwd te raken met de extra informatie die kan worden verkregen met een onzekerheidsanalyse. Er zijn echter meer inspanningen nodig voordat een onzekerheidsanalyse kan worden opgenomen in het beleid.

Summary

Risk assessment of pesticides in the Netherlands follows the EU procedure according to directive 91/414/EEC. Risk assessments in the Netherlands are carried out for active substances and formulations (products) using the computerised Uniform System for the Evaluation of Substances (USES). The measure of risk used in USES is a single-point or deterministic estimate, described by a quotient of a predicted environmental concentration and a non-extrapolated toxicity value for the organisms under consideration. A deterministic approach can be useful for a first survey, but this method does not account for the range of possible results and the fact that that some results are more likely to occur than others. Deterministic estimates may mislead decision-makers by producing falsely accurate estimates. An uncertainty analysis can be of great value for the policies of decision-makers. An uncertainty analysis accounts for the variation in the input values by incorporating their probability distributions, which leads to a probability distribution of the risk. With a probabilistic approach the full range of the resulting risk and the main sources of uncertainty are available for decision-makers. Another advantage is that it also shows the information needed to refine the risk assessment.

Example calculations are presented in this document to provide the decision-maker with additional insights concerning probabilistic risk assessments of pesticides. It is also discussed how a probabilistic analysis can be interpreted. The example calculations show that decision-makers are presented with more information to base their decisions on. In these examples, only chemical-specific uncertainties are quantified and other sources of uncertainty and variability are ignored. The registration of pesticides is directly influenced by a probabilistic analysis. The Manual for the Registration of Pesticides (CTB, 1999) presents background information about the factors by which the risk limits for the leaching to groundwater and for surface water organisms can be exceeded. For those end points, an additional model uncertainty of 100 is incorporated in the risk limits for the registration of pesticides. This factor may be reduced when a probabilistic analysis will be used. Compared to the results of the risk assessment for registration calculated with USES 1.0, the results of the uncertainty analysis with USES 3.0 are more conservative for surface water organisms and leaching to groundwater and are less conservative for earthworm. The uncertainties in the results of USES depend on the chemical properties of a pesticide. Generally, the degradation is the main source of uncertainty. Nevertheless, for the surface water end point of some example pesticides Kom, vapour pressure and water solubility are also important. For the leaching to groundwater, not only degradation but also Kom is a main source of uncertainty. The result is less sensitive for degradation when the uncertainty in the toxicity values is included. Furthermore, an option is presented for a more detailed uncertainty analysis of the effect assessment.

This document is intended for decision-makers to become acquainted with the additional information that is provided by a probabilistic analysis. Further effort will be needed before a probabilistic analysis can be incorporated into the routine assessment of pesticides.

1. Introduction

The model 'Uniform System for the Evaluation of Substances' (USES) is used in the Netherlands for the exposure assessment of pesticides (RIVM, VROM, VWS, 1999). USES is a risk assessment system which includes agricultural and non-agricultural pesticides. The model is a decision-support system to be used by central governments, research institutes and the chemical industry for rapid, quantitative assessments of the risks of pesticides. The distribution routes for the assessment of pesticides in USES are presented in Figure 1.

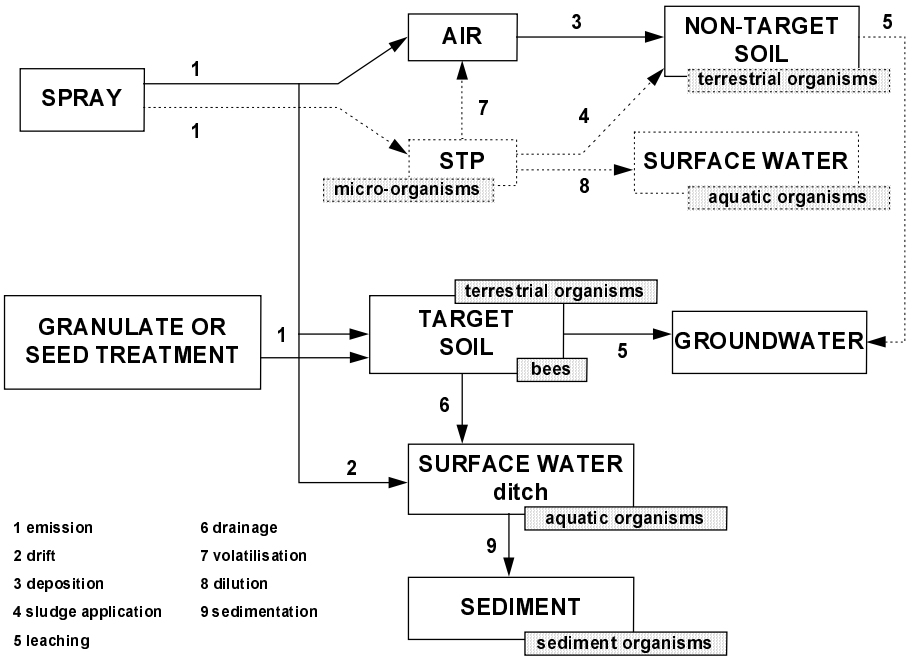


Figure 1 Distribution routes for the exposure assessment of agricultural pesticides in USES. Grey boxes contain the end points, dotted lines and boxes are used if the only release is via a sewage treatment plant.

A risk assessment can include a broad array of information sources and analysis techniques. Measured data are available for parts of the assessment of pesticides, but they can be of unknown or questionable quality. Therefore, assessors have a responsibility to present not just numbers, but also a clear and explicit explanation of the implications and limitations of the applied data. With an uncertainty analysis, quantitative information concerning this issue can be presented to decision-makers.

The most common type of modelling used in the risk assessment of substances is a deterministic approach. The assessment of pesticides in the Netherlands is also based on this approach. The deterministic approach includes a single 'best-guess' estimate of each variable within a model. For the deterministic approach, a quantitative analysis of sensitivities can be performed. In that case the effect on the outcome is examined by changing one input variable at a time while leaving the others constant. This method does not account for every possible value and the likelihood of occurrence of each variable. A quantitative assessment of the uncertainty can be performed with an uncertainty analysis. An uncertainty analysis accounts for the variation in each of the input variables by incorporating their probability distributions. With this analysis a probability distribution is assigned to each parameter after which values are randomly sampled from each distribution and inserted in the exposure equations. The random sampling is called the

Monte Carlo simulation method. Monte Carlo simulation is not the only technique to calculate the outcome of a distribution, but is the only one used for the purpose of this report.

The main goal of this study is to make decision-makers see the added value of probabilistic analysis versus the traditional deterministic approach, which hopefully can lead to a better and more defensible decision-making. With a probabilistic analysis a decision-maker can be provided with information concerning the quality of an assessment, major data gaps, and the effect that these gaps can have on the developed exposure estimates. By analogy with the studies of Jager et al. (1997, 1998, 2000 and 2001), concerning the uncertainty analysis with EUSES, the following questions will be answered:

1. How can uncertainty analysis be incorporated in the result of the assessment of pesticides (Chapter 5 and 6) ;
2. How can uncertainty be interpreted when it is incorporated in the result of the assessment of pesticides (Chapter 6 and 7).

Examples of calculations are described in chapter 6 to illustrate the added value of an uncertainty analysis versus the traditional deterministic approach. The results of an uncertainty analysis are of little value for use in the decision-making process if they are not clearly presented. This report describes the result of a probabilistic assessment of pesticides and tries to offer some guidance for evaluating these assessments for decision makers (Chapter 6 and 7). For a better understanding of the risk assessment of pesticides, the procedures in the EU and the Netherlands are explained in Chapter 3. Chapter 3 also presents recommendations concerning the use of uncertainty analysis in other international frameworks.

2. Analysis and Methods

This report discusses the results of a probabilistic risk assessment of a pesticide applied via spraying. The example pesticide is used for approximately 50 different applications in the Netherlands, but in this report, only the application in apple orchards is considered. The environmental end points are restricted to the surface water system (ditch) and the target soil, including groundwater. The data files of the example pesticide have been delivered to the RIVM for registration in the Netherlands. These data files are confidential and therefore the name of the active substance and products cannot be mentioned in this report. Nevertheless, the results of the probabilistic risk assessment can be compared with the results of the risk assessment for registration. The example pesticide was selected because it was already assessed in the Netherlands in 1999 and it is a neutral organic chemical that leaches to groundwater and poses not too many problems for USES.

For the purpose of this uncertainty analysis, the USES 3.0 equations (RIVM, VROM, VWS, 1999) were programmed in Microsoft Excel. The uncertainty analysis was carried out using Monte Carlo sampling with Crystal Ball version 4.0c, which is an add-in for Excel. The sampling was performed using the Latin-Hypercube option with 1000 runs. The detailed procedure of the uncertainty analysis, the choice of uncertainties and variabilities to be taken into account and the quantification of uncertainties are the subject of this report.

The following assumptions and simplifications were made for the uncertainty analysis of pesticides with USES:

- The analysis is restricted to uncertainty in the chemical-specific parameters (e.g. physico-chemical properties, partitioning coefficients, and degradation rates) and the uncertainty in specific parameters concerning the pesticide use (e.g. dosage, application interval).
- In this report, the uncertainty analysis will result in a probability distribution of the exposure or risk, given the selected exposure scenario (the variability of the environment is ignored) (see Section 4.1).
- Only the results of an application via spraying are taken into account. Agricultural pesticides applied via granulates, the seed treatment of pesticides, non-agricultural pesticides and the amenity use of pesticides are not taken into account;
- This study is mainly focussed on the exposure assessment, because an extensive uncertainty analysis of the effect assessment will be taken into account in another study (Roelofs, 2001). Nevertheless, in two examples of calculations, the uncertainty in the EC50 of the crustacean *Daphnia magna* and LC50 of the earthworm *Eisenia andrei* will be taken into account. In Appendix 4 recommendations are presented for implementation of uncertainty analysis in the effect assessment;
- The indirect human exposure routes, the sediment of the ditch and the exposure of bees are not taken into account for the uncertainty analysis.

3. The assessment of pesticides in the EU and other international frameworks

3.1 Procedures in the EU

In the European Union (EU), a rather complicated procedure should be followed (Council Directive of 15 July 1991, 91/414/EEC) concerning the placing of plant protection products on the market. The process started with the determination of a list of active substances registered in the EU. From a total of approximately 850 substances, 90 have been selected for the first priority list. The registrants of the active substances on this list are given a certain time to deliver a dossier to the authorities. The EU distributes all the substances on the list to the registration authorities in the Member States (MS). Based on the number of inhabitants, all Member States receive a limited number of active substances to evaluate. A Member State, indicated as Rapporteur Member State (RMS), prepares a summary of the studies required and also carries out a risk assessment for the substance based on the methodology used in that country and reports in a so-called monograph. The draft monograph is discussed in an ECCO-meeting (ECCO = European Commission Co-Ordination) for peer review on five subtopics. In an integration meeting all the topics come together and a proposal is prepared for discussion in the Standing Committee on Plant Health (SCPH). Before decision making, the draft monograph is also presented to the registrant for additional comments and possible additional information. A registrant may want to discuss the monograph with the authorities in a tripartite meeting. Also the need for additional data can be discussed with the registrant. The SCPH asks the Scientific Committee on Plants (SCP) for advice on the scientific soundness of the monograph and the conclusions. Finally, the SCPH takes a decision on the inclusion of the active substance on Annex I of Directive 91/414/EEC. A positive decision means that, in principle, there is a safe use of the active substance possible in the EU and therefore the active substance may be marketed in the EU. If the decision of the SCPH is negative the substance is not allowed for use in the EU. A third option can be a postponement of the decision if additional information is required. After the substances have been put on Annex I, each MS has to carry out a risk assessment with the substance in the product for which authorisation is wanted. The product evaluated in the EU to receive Annex I listing may be a different product compared to the product in another country due to differences in the formulation.

The items relevant to the environmental evaluation of the active substance are generally the same as in many countries. Some differences may however occur. In the EU the following items have to be evaluated from an environmental point of view:

- Persistence in soil;
- Leaching to groundwater;
- Effects on terrestrial vertebrates;
- Effects on water organisms, including bioaccumulation;
- Effects on bees and other arthropods;
- Effects on earthworm and other soil macro-organisms;
- Effects on soil micro-organisms;
- Effects on other non-target organisms;
- Effects on biological methods of sewage treatment.

For the EU risk assessment, a deterministic approach is chosen; an uncertainty analysis is not performed in this framework. The risk assessment is based on the TER-value, which stands for Toxicity over Exposure Ratio. Because of the definition, it is the opposite of the PEC/PNEC-value, which is the ratio of the exposure over a single-specie toxicity value that is extrapolated to the population or ecosystem level, the Predicted Environmental Concentration (PEC) over the Predicted No-observed Effect Concentration (PNEC). If the TERs are below a certain trigger-value, higher tiers of risk assessments have to be considered for exposure and / or toxicity to determine whether there is still a risk. In principle, the registrant may continue to raise additional information on the topics showing risk. The decision system does not end with a final approval or rejection of the product. Only if the company does not want to spend more effort to raise additional information, the substance may be withdrawn from the market. The same may occur on the national level.

3.2 Procedures in the Netherlands

The assessment of pesticides in the Netherlands is closely related to the EU procedure. In this framework also no uncertainty analysis is performed. For registration of a pesticide in the Netherlands, the European procedure must be followed according to directive 91/414/EEC. If the Netherlands acts as Rapporteur Member State (RMS), not only an EU monograph is prepared but the pesticide is also assessed for registration in the Netherlands. The Netherlands comment on EU monographs if it is not a RMS and in that case the pesticide is only assessed for possible risks in the Netherlands when the registrant is applying for registration. In the Netherlands, these evaluations and risk assessments are carried out for active substances and formulations (products) with the computerised USES (Uniform System for the Evaluation of Substances). USES generates risk characterisation ratios (RCR), described by a quotient of a predicted environmental concentration (PEC) and a non-extrapolated toxicity value for the organisms under consideration.

To determine the PEC values, USES makes use of advanced models like PEARL and TOXSWA (see Section 4.2). Generally, the risk assessment is carried out at the level of the organism rather than on the level of the ecosystem, which is in agreement with the EU-approach. The PEC values established with USES are the basis for the risk assessment in the Netherlands. Sometimes, if there are special circumstances, the concentrations may be adapted to the situation under consideration, e.g. in case of risk management or risk reduction due to special agreements between the authorities and the companies or farmers. With some adjustments, the data generated with USES are incorporated in the evaluation and risk assessment of the active substance under consideration. One example of an adjustment is the dose of 1 kg/ha, which is used in USES to calculate the leaching potential. In the evaluation the correct dose as given on the label is used by multiplying the result of USES with the actual dose. The calculated RCRs are used to determine the necessity of additional data to be provided by the applicant of the substance if the trigger value of the organism under consideration is exceeded. The applicant must provide additional data. If the trigger value of the item under consideration is not exceeded, the substance meets the criteria for that part of the evaluation.

3.3 Uncertainty analysis in other programs

Actually, there are no models or programs for pesticides reported in the literature that are comparable to USES. Some programs are not computerised nor provide a complete overview of all the items of a risk assessment for pesticides. However, the following three programs should be mentioned, in relation to the uncertainty analysis of the assessment of pesticides.

1. ECOFRAM in the USA;
2. ERA of EPPO;
3. FOCUS of the EU.

3.3.1 ECOFRAM

ECOFRAM, Ecological Committee On FIFRA Risk Assessment Methods, consists of two working groups, one on terrestrial and one on aquatic ecotoxicology. The results of the work of the ECOFRAM working groups has been published in two reports with recommendations to the Environmental Protection Agency (EPA) in the US to improve the risk assessment methodology. One of the main recommendations of both groups was the further development of probabilistic risk assessment methods providing decision-makers with an easier to use decision-making criterion compared to the present deterministic approach. Currently EPA is considering whether to follow the recommendations of the ECOFRAM working groups. Whatever the decision will be, it should be clear that, even though the methods are in principle available, a lot of development has to be carried out before uncertainty analysis can be implemented to its fullest extent in risk assessment (ECOFRAM, 1999).

Several models are used in the US to determine the exposure concentration in environmental compartments, like PRZM, EXAMS, and GENEEC. Only PRZM is specifically designed for the assessment of pesticides. Although several of these models have been validated and used for some time, no uncertainty analysis has been carried out. It is unclear if uncertainty analysis will be incorporated in the future.

3.3.2 ERA

The Environmental Risk Assessment (ERA) schemes of the joint panel of the European and Mediterranean Plant Protection Organisation (EPPO) and the Council of Europe (CoE) have been developed in the early nineties. The schemes address three environmental compartments: soil, groundwater and surface water. The compartment air was not considered. In addition to the environmental compartment, a risk assessment method was presented for several organisms: terrestrial vertebrates, aquatic organisms, earthworm, bees, soil microflora and arthropod natural enemies. The schemes have been published in a special issue of the EPPO Bulletin (Volume 23 and 24, 1993 and 1994, respectively). In an additional chapter, some remarks were included on the item of uncertainty analysis. It identified the sources of uncertainty in a risk assessment procedure:

- errors in measurements (of ecotoxicity, environmental concentrations, etc.);
- extrapolation from species to species or case to case and other cases which require expert judgement;
- assumptions (e.g. on the depth of soil that is relevant to earthworm) and arbitrary thresholds, which may be used as triggers for further tests.

The sources of uncertainty could result in 'false negatives' and 'false positives'. It was stressed that both types of errors should be minimised. In addition it was suggested to run through the schemes several times with different values of some key parameters to get some feeling for the variation in the outcomes. This activity can give an entry to perform an actual quantitative uncertainty analysis.

During a succeeding workshop (11-13 June 1997 in Bilthoven, the Netherlands) participants were asked to carry out risk assessments for 5 dummy pesticides according to the methods used in the participating countries. The wide variety in the results of the risk assessments of the different countries showed that the guidance was unclear. Therefore, the results were not used with the specific intention of an uncertainty analysis but more as a test to come to an improvement of the schemes. The schemes are currently being updated but the uncertainty analysis will not be incorporated. Again uncertainty analysis will be included in a chapter of the EPPO bulletin, albeit more elaborate than in the 1993-issue.

3.3.3 FOCUS

The Forum for the co-ordination of pesticide fate models and their use (FOCUS) first made inventories of existing models for soil, leaching and surface water. In addition, and based on the inventories, European scenarios have been developed for groundwater and are under development for surface water. For groundwater the existing models MACRO (SE), PEARL (NL), PELMO (GE), and PRZM (US) are used to estimate the concentration in groundwater. In the report of the working group on groundwater scenarios a separate chapter is devoted to uncertainty issues. Uncertainties are considered related to:

- calculation and interpretation of results;
- model choice and model parameterisation;
- choice of scenarios;
- input and
- interpretation of output.

Proposals are presented to reduce the uncertainty by reviewing the suitability of the selected scenarios, data set improvement, and comparison of model results. In this framework, no actual uncertainty analysis has been carried out, although the item is mentioned as a follow-up activity (FOCUS, 2000).

Considering surface water, the final report on the scenario selection is not yet ready. It is expected to be ready at the end of 2001, but no uncertainty analysis will be included. As for groundwater only a chapter will be presented with sources of uncertainty and some recommendations to overcome or to minimise the uncertainty. At the moment, it is too early to anticipate on these results.

4. Uncertain parameters

4.1 Uncertainty and variability

Uncertainty represents a lack of knowledge about specific factors or parameters that characterise the physical system that is being modelled and includes parameter uncertainty (e.g. measurement errors), model uncertainty (e.g. uncertainty due to necessary simplifications) and scenario uncertainty (e.g. descriptive errors). Uncertainty can lead to inaccurate or biased estimates and can be reduced through further measurements with for instance a larger sample size, an unbiased sample design, or with more appropriate target species. The use of more sophisticated modelling and analysis tools can also reduce uncertainty. The above-mentioned uncertainty arises due to a lack of knowledge of model-parameter values. In fact, these parameter values are deterministic, but the actual value can not be determined accurately. Variability is another type of uncertainty and refers to observed differences due to heterogeneity or diversity in a population or differences between ecosystems in structure, sensitivity or exposure level. In other words, variability is the effect of chance and is a function of the system. Unlike uncertainty, variability is usually not reducible by further measurements or study. Total uncertainty is the combination of uncertainty and variability.

This report tries to distinguish between variability and uncertainty. As has been mentioned above, further study or measurements can only reduce uncertainty, not variability. Therefore, separating uncertainty and variability is necessary to identify parameters for which additional data are needed (EPA, 1997). Furthermore, when uncertainty and variability are mixed together, information is lost in knowing what component of the result is due to inherent randomness (variability) of the system, and what component is due to our ignorance of the environment (Vose, 2000). Uncertainty may force decision-makers to judge how probable it is that exposures have been over- or underestimated. Variability forces them to cope with the certainty that different individuals are exposed both above and below any of the exposure levels chosen as a reference point (EPA/ORD/NCEA, 1997). This analysis is restricted to uncertainty in the chemical-specific parameters (e.g. physico-chemical properties, partitioning coefficients, and degradation rates). The uncertainty in specific parameters concerning the pesticide use (e.g. dosage, application interval) are not taken into account (see Appendix 3). The characteristics of the environment are defined as ‘scenario properties’, thereby ignoring the variability in them.

In many cases the distinction between the above mentioned uncertainty in parameters and variability in scenario properties is not completely straightforward. Parameters can depend upon properties of the chemical as well as on properties of the environment. This can be illustrated by for instance biodegradation which, apart from being a chemical-specific parameter, also depends on variable properties like soil temperature or available bacterial populations (Jager, 1997). It should be noted that generally the variability component is more important than the uncertainty component.

The risk assessment for pesticides in the Netherlands is not performed for an existing location but for a so-called standard environment by using a reasonable worst-case exposure scenario. The variability of this scenario is very difficult to quantify. For example, a pesticide applied via spray can end up in a ditch. The ditch size and the pesticide concentration vary between locations and even in time. Also the exposed aquatic organisms in a ditch are not always at the same spot in the ditch. When the generally dominant natural variability is ignored, the assessment can be judged in a more transparent manner, although the relevance of the analysis

decreases. In this report, the uncertainty analysis will result in a probability distribution of the exposure or risk, given the selected exposure scenario where the variability of the environment is ignored.

4.2 Choice of distribution routes

The application of pesticides can occur through spraying of the substance and through application of granules or treated seeds. For this study, only the application through spraying of a pesticide is taken into account. For this application the distribution routes are:

1. Emission to the target soil
2. Drift to surface water (ditch)
3. Leaching from target soil to groundwater
4. Sedimentation from surface water (ditch) to sediment

These routes are presented in Figure 2. In this figure, the boxes in the lower right corner of each environmental compartment contain the end points for the application of a pesticide via spray. For the uncertainty analysis, only the boxes (environmental compartments and end-points) with black frames are taken into account, that are connected by the distribution routes 1-3.

The indirect human exposure via groundwater is not used, because this route is a part of the total dose that is combined with other intake routes that are not taken into account in this report. The sediment of the ditch has been left out, because this compartment was not assessed for the example pesticide mentioned in Chapter 6. The uncertainty analysis was not focussed on the assessment of bees and therefore this end point was also not taken into account. Within the USES 3.0 model, the atmospheric compartment is only used for non-target soil end points and is therefore less relevant for this study.

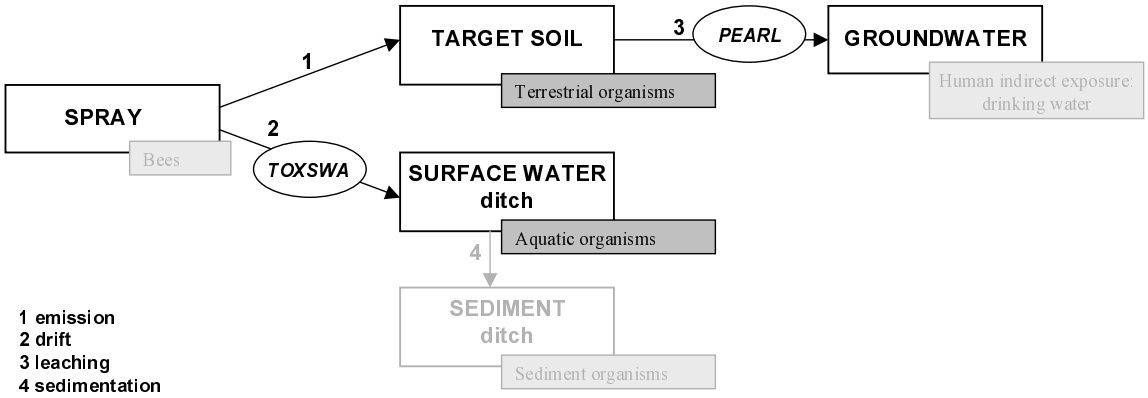


Figure 2 Distribution routes for the application of pesticides through spray. The grey boxes contain the end points. In this report only the boxes with black frames are taken into account, that are connected by the distribution routes 1-3.

The (meta)models of PEARL and TOXSWA are included in Figure 2. For single compounds a metamodel based on the PEARL model (Leistra et al., 2000) is used in USES 3.0 to calculate the concentration in the upper groundwater (1 to 2 meter depth). PEARL is an acronym for Pesticide Emission Assessment at the Regional and Local scale. In the pesticide registration a standard scenario is used for calculating the leaching potential of a substance applied in spring (26 May)

and/or autumn (1 November). The input, needed to run the metamodel, is the half-life of the substance under reference conditions (DT50) and the sorption constant normalised to organic matter (Kom). The results derived from the metamodel are incorporated in USES 3.0 as interpolation tables for spring and autumn.

The concentration in surface water is calculated using a metamodel of the TOXSWA model (Adriaanse, 1996). TOXSWA is an acronym for TOXic substances in Surface WAters. This model describes the fate of pesticides entering water bodies. In the Dutch standard scenario, TOXSWA simulates single or repeated loading via spray drift. The standard results derived from the metamodel for a spring and autumn application are incorporated in USES 3.0 as tables for each exposure duration, number of applications, application interval and half-life of the substance under standard conditions (DT50). The concentration in the sediment is calculated using equilibrium partitioning between water and sediment. Possible accumulation of pesticides in the sediment layer of the surface water compartment is taken into account as well.

4.3 Choice of uncertain parameters

For the distribution routes, mentioned in Section 4.2, a flow chart and all parameters used are presented in Appendix 2. As has been mentioned in Section 4.1, uncertain and variable parameters have to be separated from each other and are marked in Appendix 2. For each distribution route the selected parameters are presented in Table 1. For these parameters, the characteristics of the distributions are explained in Chapter 5.

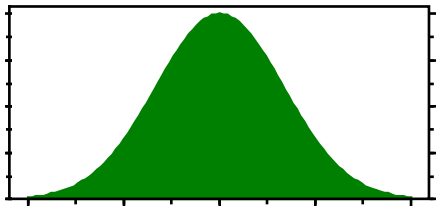
Table 1 The selected parameters for each distribution route of the USES 3.0 program.

Symbol	Description	Unit
Surface water ditch:		
VP	Vapour pressure	[Pa]
SOL	Water solubility	[$kg_c.m^{-3}$]
HENRY	Henry's law constant	[$Pa.m^3.mol^{-1}$]
Kow	Octanol-water partitioning coefficient	[-]
$kdeg_{water,temp}$	Temp dependent rate constant for degradation (=ln2/$DT50_{water}$)	[d^{-1}]
Koc	Organic carbon-water partitioning coefficient	[$m^3.kg^{-1}$]
Kom	Organic matter-water partitioning coefficient	[$m^3.kg^{-1}$]
TOXSWA	Tables (see reference: RIVM, VROM, VWS, 1999; appendix VIII)	[$\mu g.l^{-1}$]
$Kaw\text{-}pest_{water}$	Partial mass transfer coeff at water side of the air-water interface	[$m.d^{-1}$]
$Kaw\text{-}pest_{air}$	Partial mass transfer coeff at air side of the air-water interface	[$m.d^{-1}$]
Sediment ditch:		
Koc	Organic carbon-water partitioning coefficient	[$m^3.kg^{-1}$]
Kom	Organic matter-water partitioning coefficient	[$m^3.kg^{-1}$]
Target soil:		
VP	Vapour pressure	[Pa]
k bio_{soil}	Rate constant for biodegradation in soil (=ln2/$DT50_{bio,soil}$)	[d^{-1}]
k $abio_{soil}$	Rate constant for abiotic degradation in soil (=ln2/$DT50_{abio,soil}$)	[d^{-1}]
Groundwater:		
VP	Vapour pressure	[Pa]
Kom	Organic matter-water partitioning coefficient	[$m^3.kg^{-1}$]
k bio_{soil}	Rate constant for biodegradation in soil (=ln2/$DT50_{bio,soil}$)	[d^{-1}]
k $abio_{soil}$	Rate constant for abiotic degradation in soil (=ln2/$DT50_{abio,soil}$)	[d^{-1}]
PEARL	Tables (see reference: RIVM, VROM, VWS, 1999; appendix VII)	[$\mu g.l^{-1}$]

5. Probability distributions

Probability distributions must be defined for the uncertain parameters. The difficulty of selecting appropriate parameter distributions may be reason for lack of acceptance of probabilistic risk assessment among regulators (Finley and Paustenbach, 1994). The final distribution of risk may depend strongly upon the shape and magnitude of the input distributions but, nevertheless, even limited information about the distribution of an input parameter is better than assuming a single value for an entire population (Anderson and Yuhas, 1996).

5.1 The normal distribution



The normal distribution is probably the most popular distribution since many natural phenomena like people's height can be satisfactory described by it. The distribution is symmetrical and extends from minus infinity to plus infinity. The normal distribution is characterised by a mean and a standard deviation. As a rule of thumb, approximately 68% of the values are within one standard deviation from the mean and 95% within 2 standard deviations.

The results in this report will be presented in cumulative probability distribution figures, which are derived from probability density plots (Figure 3). The advantage of cumulative probability plots is that the probability that a Risk Characterisation Ratio (RCR) is lower than 1 can be read directly from the value found on the y-axis. A more obvious parameter to focus on is the probability that RCR exceeds one, which is 100% minus this value.

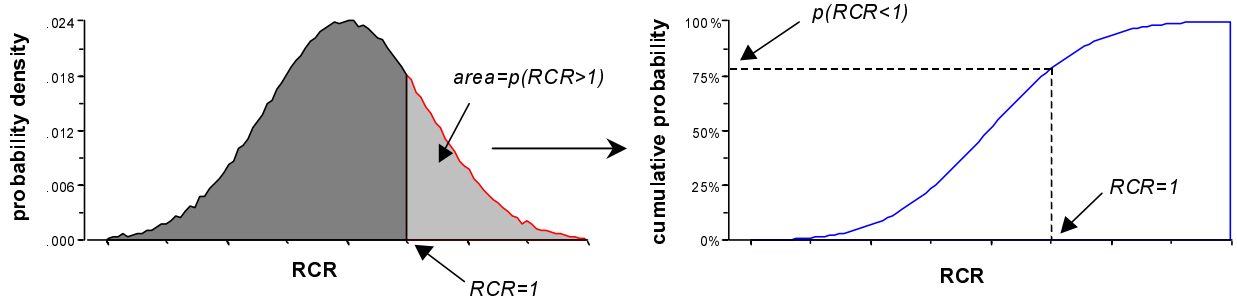
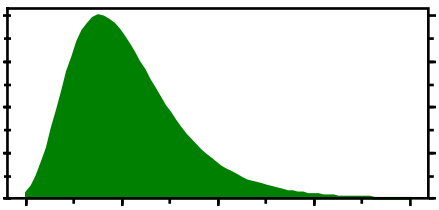


Figure 3 Relation between a relative and a cumulative probability plot

5.2 The lognormal distribution



There are strong theoretical and empirical considerations to assume a lognormal distribution *a priori* for many physical entities (Slob, 1987; Seiler and Alvarez, 1996). The lognormal distribution is positively skewed, and has a domain ranging from zero to infinity. These properties make the lognormal distribution less suited for parameters which have a physical upper limit like fractions which are usually smaller than 1. The distribution can be characterised by the median and a measure for the variation. A convenient measure is the 'dispersion factor' or k which is defined as follows: 95% of the values is within a factor of k from the median (Slob, 1994). This dispersion factor has the advantage of being readily interpretable and can be simply related to the standard deviation or coefficient of variation (Slob, 1994; Jager, 1997).

5.3 Parameter distribution for USES 3.0

In order to describe the uncertainty in the model output, the uncertainty in the model input parameters has to be quantified. This was done by analysing parameter measurements of 28 pesticides from the Mackay (1999) database and the ARS Pesticide Properties database (see Appendix 3). The data from these databases are used to quantify the parameter distributions, and are not evaluated according to the criteria for the registration of pesticides. Therefore, the retrieved distributions can deviate from those expected to be found according to the registration of pesticides. For the purpose of this report, the distributions of existing substances mentioned in Jager et al. (1997) were not adopted, but new parameter distributions for pesticides are derived. Several measured values were available for each parameter and each pesticide. The distributions for all parameters appeared to be lognormal, except for the effect-parameters that were normally distributed. For each pesticide, the median parameter value was calculated. Also, the deviation from the median was calculated for each pesticide. The deviations from the median are shown in the residual plots in Appendix 3. The dispersion factor (k) was then calculated for each pesticide:

$$k = \exp(1.96\sigma_{resid}\ln b)$$

k = dispersion factor
σ_{resid} = standard deviation of the residuals on log scale
b = the base of the logarithm that was used to calculate the standard deviation

By visual judgement, cut-off values were chosen in the residual plots when deviations from the median value were not in the same order of magnitude for the 28 pesticides. A mean dispersion factor was calculated for each group of pesticides. The dispersion factor and the type of distribution for several input parameters is summarised in Table 2. Simple correlation coefficients were calculated between Kow-solubility, Kow-vapour pressure, Kow-Henry's law constant, and Kow-Koc by taking the average values on log scale. The correlation coefficient between Kow and vapour pressure was not significant (see Appendix 3). In Appendix 3 the derivation and quantification of the distributions of the chemical specific parameters are described.

Table 2 Summary of the parameter distributions for the USES 3.0 model.

Parameter	Symbol	Type of distribution *)	Remarks
Physico-chemical properties	All data from; Mackay (1999) and the ARS Pesticide Properties Database		
Octanol-water partitioning coefficient	Kow log Kow ≤ 3.4 log Kow > 3.4	 k=4.3 (L, n=18) k=30.2 (L, n=9)	Different uncertainty for low and high *Kow* values.
Water solubility	SOL SOL ≤ 15 mg/L SOL > 15 mg/L	 k=8.7 (L, n=7) k=1.8 (L, n=21)	Different uncertainty for low and high solubility. Correlated to uncertainty in *Kow*, (corr. Coeff.= -0.91 on log scale).
Vapour pressure	VP VP ≤ 0.01 Pa VP > 0.01 Pa	 k=6.8 (L, n=21) k=3.0 (L, n=7)	Different uncertainty for low and high vapour pressure. Correlation to *Kow* was not significant.
Partitioning coefficients			
Organic-carbon normalised partitioning coefficient	Koc	k=5.1 (L, n=26)	Correlated to uncertainty in *Kow*, (corr. Coeff.= 0.92 on log scale).
Henry's law constant	HENRY HENRY ≤ 0.03 HENRY > 0.03	 k=83.3 (L, n=17) k=5.5 (L, n=9)	Only relevant when measured. Correlated to uncertainty in *Kow*, (corr. Coeff.= 0.71 on log scale).
Biodegradation rates			
Biodegradation rates in surface water and soil	$DT50_{water}$ $DT50_{soil}$	k=17.1 (L, n=23) k=8.5 (L, n=27)	
Effect concentrations			
Daphnia magna	EC50 mg/l	N[1)] (M=85.3 ± 5.7 95% conf. Int.)	Only applicable to the sample pesticide (see Chapter 6)
Eisenia andrei	LC50 mg/kg	N[1)] (M=10.7 ± 1.95 95% conf. Int.)	Only applicable to the sample pesticide (see Chapter 6)

*) L=Lognormal
N=Normal. Defined by a mean (M) and 95% confidence limits.

1) These normal distributed data were mentioned in the available dossier of the sample pesticide. Usually an analysis is performed on log-transformed concentrations that leads to skewed confidence intervals.

6. Examples of calculations

In this chapter, examples of calculations are presented to illustrate the added value and potential of an uncertainty analysis versus the traditional deterministic approach. Also, it will be discussed how a probabilistic risk assessment can be interpreted when it is incorporated in a risk assessment. The examples of calculations are based on two approaches:

1. A pesticide that has been assessed for registration in the Netherlands is used as an example pesticide (called example pesticide throughout the report). The results of the probabilistic risk assessments are compared with the deterministic quotient approach[1]. In two examples of calculations, deterministic toxicity data is used and two additional calculations use uncertain toxicity data;
2. Results of five other pesticides are compared with results of the example pesticide, in order to generalise the results from the example pesticide. A probabilistic exposure assessment is executed for a ditch, target soil and groundwater. For this example, no toxicity data are used.

For each end point the main source of uncertainty is presented. In addition, the log RCR value or log concentration is presented in tables, where the deterministic and the probabilistic approach are compared. The data of the example pesticide are taken from the confidential report of the risk assessment, on which the registration by the Pesticides Authorisation Board (CTB) is based. In this 1999 report the calculations were performed with USES 1.0. Therefore, the results of the uncertainty analysis of USES 3.0 are compared with the USES 1.0 results. The table format, used to present the results of the uncertainty analysis, is explained in Table 3.

Table 3 Explanation of the table format used to present the results of the deterministic and probabilistic approach.

	End points
Deterministic	
USES 1.0 log RCR or log concentration	Result calculated with settings for the example pesticide in USES 1.0, as mentioned in the report of the risk assessment for registration
USES 3.0 log RCR or log concentration	Result calculated with the standard USES 3.0 settings
Probabilistic	
50 %	50^{th} percentile of the risk estimates distribution. This is the median risk level.
90 %	90^{th} percentile of the risk estimates distribution
95 %	95^{th} percentile of the risk estimates distribution
USES 1.0 percentile	The percentile of the risk distribution which equals the risk estimate as given by the settings for the example pesticide in USES 1.0, as mentioned in the report of the risk assessment for registration
USES 3.0 percentile	The percentile of the risk distribution which equals the risk estimate as given by USES 3.0

[1] The risk assessment of pesticides includes the use of a so-called quotient approach to estimate risk. A quotient is an index of risk calculated by dividing an exposure estimate by a toxicity reference value (e.g. LC50, NOEC). The numerator and denominator values are in the same exposure units so that the ratio is dimensionless. The type of toxicity value depends on the end point (see Figure 2).

6.1 Approach 1

In this section, the probabilistic results are compared with the deterministic quotient approach. For the pesticide that has been assessed for registration (February 1999), the results are compared with the deterministic quotient approach according to the following four examples of calculations:

A. Uncertain exposure concentration in **surface water (ditch)**, with deterministic toxicity. Four end points: algae (NOEC), Daphnia (LC50), Daphnia (NOEC) and fish (LC50)
B. Uncertain exposure concentration in **target soil / food (bird)** with deterministic toxicity. Three end-points: earthworm (LC50), bird food (LD50 – Colinus 1), bird food (LC50 – Colinus 5)
C. Uncertain exposure concentration in **surface water (ditch)** with uncertain toxicity. End point: Daphnia (LC50)
D. Uncertain PEC for **target soil** with uncertain toxicity End point: earthworm (LC50)

A. Surface water (ditch) and deterministic toxicity

The results are presented in the cumulative probability distributions and sensitivity chart of Figure 4. On the left-hand side of this figure the deterministic RCR values that were calculated with the quotient approach (USES 3.0) are indicated with short vertical bars, together with the cumulative probability of RCR values. RCR values are presented on log scale, where log RCR = 0 is equivalent to RCR = 1. Similarly, log RCR = -2 is equivalent to RCR = 0.01. The influence of each input parameter on the end point distribution is indicated in the sensitivity chart on the right-hand side of figure 4. Daphnia 0 (0 days) is the short term RCR for the crustacean Daphnia and Daphnia 21 (21 days) is the long term RCR. The sensitivity chart for Daphnia is shown only, since the charts for the other end points are very similar.

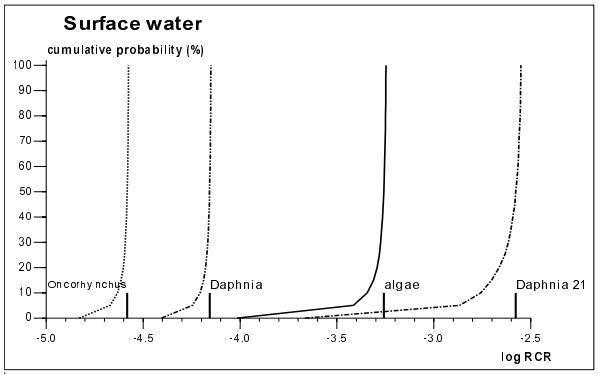


Figure 4 Cumulative probability of RCR values for four end points and sensitivity chart for Daphnia. Daphnia 0 (0 days) indicates the short term RCR for the crustacean Daphnia and Daphnia 21 (21 days) is the long term RCR. The deterministic RCR values for each end point that were calculated with the quotient approach (USES 3.0) are indicated with short vertical bars on the x-axis of the left figure. The influence of the input parameters on the RCR for the end point Daphnia is indicated in the sensitivity chart of the right figure.

The cumulative distributions of the Risk Characterisation Ratios (RCR) in the surface water compartment (Figure 4) are not sigmoidal like the curve presented in Figure 3. The right-hand tail is missing. This is probably due to the fact that the end of the TOXSWA table is reached. Values for $DT50_{water}$ beyond 1000 days are not included in this table. With an uncertainty factor

of 17.1 (Table 2), it is not unlikely that with a mean $DT50_{water}$ of 113 days for the example pesticides, the end of the table will be reached. Therefore, RCR values at the right side of the sigmoid (with higher concentrations due to longer degradation rates) are missing. This effect becomes dominant because according to the sensitivity analysis, the $DT50_{water}$ parameter contributes most to the end point uncertainty. The left-hand tail of the distributions are longer for algae and Daphnia (21 days), than for fish (Oncorhynchus) and Daphnia (0 days). In the USES 3.0 model, the risk characterisation ratios for Algae and Daphnia 21 are calculated from pesticide concentrations in water after 4 and 21 days of pesticide addition, respectively. Due to degradation during this period, low pesticide concentrations are also present, which causes a longer left-hand tail.

Overall, the slope of the sigmoid is steep, which means that there is only a small uncertainty in the risk for the presented organisms, or group of organisms, if the distributions of the selected input parameters (see Table 2) are taken into account. However, this is actually not a realistic situation, because only the uncertainty of the parameters mentioned in Table 1 was taken into account. The uncertainty and variability in many other input parameters was ignored, because they were assumed to be a property of the selected scenario (see Section 4.1).

The criteria for the registration of pesticides are described in the Manual for the Registration of Pesticides (CTB, 1999). Although criteria have not yet been set for a probabilistic approach, the deterministic log RCR has been used for comparisons reasons. The presented probability plots are below the critical log RCR of –2 for fish (Oncorhynchus) and Daphnia (0 days) and below a log RCR of –1 for algae and Daphnia (21 days). For the example pesticide the aquatic risks are low, because the complete distributions for the mentioned end points are well below the critical log RCR values. The benefit of a probabilistic risk assessment is higher if the probability plots are around the critical log RCR value, because then it can be judged how much the RCR must change to obtain an acceptable risk estimate (see calculation D). The main sources of uncertainty are presented in the sensitivity chart of Figure 4. With a deterministic toxicity value the degradation ($DT50_{water}$) is the main source of uncertainty.

The results are not only presented graphically but are also explained in Table 4. This table shows that the deterministic RCR values of USES 3.0 were similar to the 50 percentile values of the distribution, or the median risk level. The reason for this is because the $DT50_{water}$ parameter is the only input parameter that contributes to the uncertainty in the risk levels (Figure 4). The median value of the $DT50_{water}$ distribution is then similar to the deterministic value of $DT50_{water}$ in the model. Therefore, the median value of the risk level distributions is also similar to the deterministic risk levels. If, however, more input parameters are contributing to the uncertainty in the risk levels, it becomes more unlikely that the deterministic risk levels are similar to the median risk levels of the distribution (see also Table 11 and Table 12). The deterministic risk levels, calculated with USES 1.0, as mentioned in the report of the risk assessment on which the registration by the Pesticide Authorisation Board (CTB) is based, are almost equal to the USES 3.0 results. Nevertheless, the USES 1.0 results are out of range of the very narrow USES 3.0 distributions. The low USES 1.0 percentiles in Table 4 (2.5 % for Daphnia and 7.5 % for algae), indicate that the USES 3.0 results are more conservative than the results of the risk assessment for registration. It is not easy to explain the reason for this difference, mainly because of the difference between the fate models of the ditch of USES 1.0 and USES 3.0.

Table 4 Results of the deterministic and probabilistic approach for calculation A: surface water (ditch) with deterministic toxicity. See Table 3 for explanation.

	Daphnia 0	Daphnia 21	Algae	Oncorhynchus
Deterministic				
USES 1.0 log RCR	-4.30	-2.96	-3.37	-4.72
USES 3.0 log RCR	-4.16	-2.58	-3.26	-4.58
Probabilistic				
50 % log RCR	-4.16	-2.58	-3.26	-4.58
90 % log RCR	-4.15	-2.55	-3.25	-4.58
95 % log RCR	-4.15	-2.55	-3.25	-4.58
USES 1.0 percentile	2.5	5.0	7.5	2.5
USES 3.0 percentile	50.0	50.0	50.0	50.0

B. Target soil (earthworm) / Food (bird) and deterministic toxicity

The results are presented in the cumulative probability distributions and sensitivity chart of Figure 5. Three end points are presented in the cumulative probability distribution figure: earthworm (LC50), bird food (LD50 – Colinus 1), bird food (LC50 – Colinus 5). Only the sensitivity chart for Eisenia is shown, since the charts for the other end points are very similar.

The slope of the cumulative probability graph is an indication for the uncertainty. Similar to the previous example, the steep slope is an indication for a small uncertainty in the soil end points. Here, $DT50_{soil}$ contributes most to the end point uncertainty. Again, the right-hand tail of the sigmoid is missing in these distributions, which is probably caused by the exponential fraction of the concentration remaining in soil after a certain time period (Frs, see equation P-93; RIVM, VROM, VWS (1999)). At smaller $DT50_{soil}$ values the parameter Frs shows some change, but rapidly reaches the value 1 at higher $DT50_{soil}$ values.

The presented probability plots for bird food (Colinus 1 and 5) are well below the critical log RCR of –1 and therefore the risk is considered low. Based on the risks of earthworm (Eisenia) the substance can be registered if it complies with the following criteria (CTB, 1999):

- It is out of the question that the substance will end up on the soil surface;
- The PEC0/LC50 < 0.001;
- 0.001 ≤ PEC0/LC50 < 0.1, the DT90 < 100 days and there are ≤ 3 applications per season;
- 0.001 ≤ PEC0/LC50 < 0.1 and the PEC/NOEC < 0.2.

For this example with a deterministic toxicity value, the complete distribution for the end point earthworm complies with 0.001 ≤ PEC0/LC50 < 0.1 (or –3 ≤ logRCR < –1). For this pesticide the $DT50_{soil}$ is higher than 100 and therefore the DT90 can not be smaller than 100 days. No NOEC was available in the risk report for registration and therefore the risk could not be determined. Here, a sublethal toxicity test is needed to determine actually the risk and whether the pesticide can be registered.

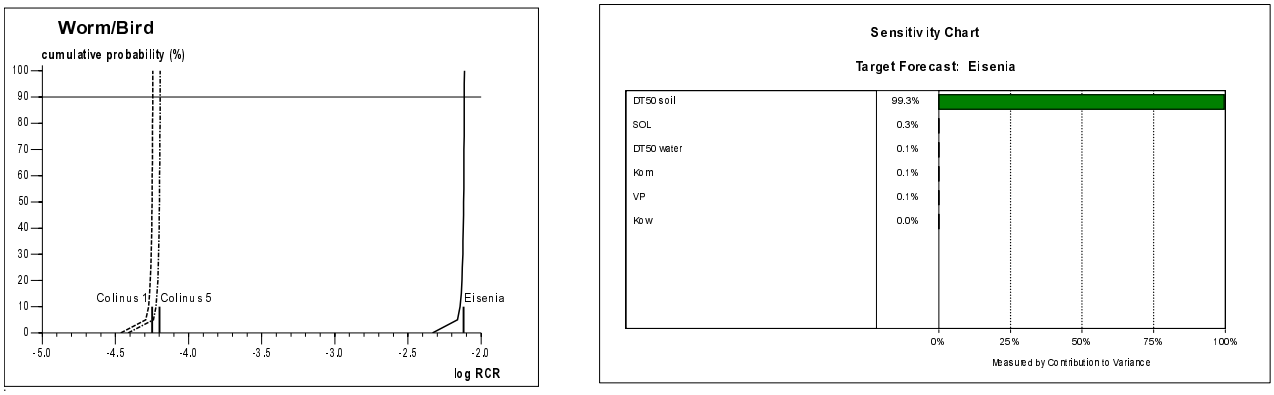


Figure 5 Cumulative probability of RCR values for three end points and sensitivity chart for Eisenia. The deterministic RCR values for each end point that were calculated with the quotient approach (USES 3.0) are indicated with short vertical bars on the x-axis of the left figure. The influence of the input parameters on the end point earthworm (Eisenia) is indicated in the sensitivity chart of the right figure.

Deterministic RCR values were similar to the 50 percentile values of the distribution, or the median risk level (Table 5). Here, compared to the results with USES 1.0, the calculated risk level for earthworm (Eisenia) was lower when calculated with USES 3.0. Therefore, for earthworm the USES 3.0 results are less conservative than the results of the risk assessment for registration.

Table 5 Results of the deterministic and probabilistic approach for calculation B: target soil with a deterministic toxicity. See also explanation in Table 3.

	Eisenia	Colinus 1	Colinus 5
Deterministic			
USES 1.0 log RCR	-2.03	n.a.	n.a.
USES 3.0 log RCR	-2.12	-4.25	-4.20
Probabilistic			
50 % log RCR	-2.12	-4.25	-4.20
90 % log RCR	-2.11	-4.25	-4.19
95 % log RCR	-2.11	-4.24	-4.19
USES 1.0 percentile	100.0	n.a.	n.a.
USES 3.0 percentile	50.0	50.0	50.0

n.a. not available

C. Surface water (ditch) with uncertain toxicity

If toxicity (LC50) for Daphnia was added to the uncertain parameters, then uncertainty in the risk quotient increased (Figure 6). The distribution becomes more sigmoidal, because $DT50_{water}$ is not the only parameter anymore that contributes to the uncertainty in the end points. Similar to calculation A, the presented probability plots are well below the critical log RCR of –2 for Daphnia (0 days) (CTB, 1999). Again, for this calculation the risk is low for Daphnia, because the complete distributions are well below the mentioned critical log RCR value.

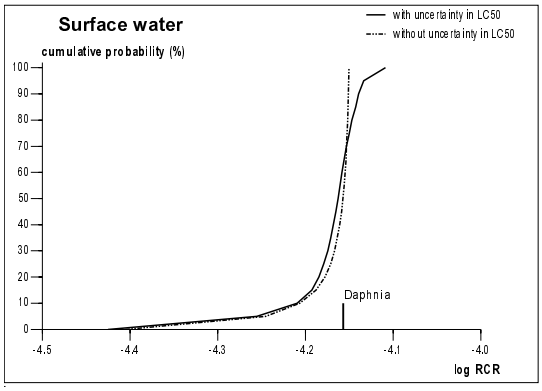


Figure 6 Cumulative probability distribution for the risk quotient of Daphnia with and without uncertainty in the LC50. The deterministic RCR value for this end point that was calculated with the quotient approach (USES 3.0) is indicated with a short vertical bar on the x-axis.

The main sources of uncertainty are presented in Table 6. The $DT50_{water}$ is the most important parameter, when uncertainty in LC50 is ignored. With uncertainty in the toxicity, both $DT50_{water}$ and $LC50_{Daphnia}$ contributed equally to the uncertainty in the RCR. The contribution of the $LC50_{Daphnia}$ is low compared to calculation D, which is a result of the low standard deviation of the aquatic toxicity test. In this example, degradation becomes less relevant if the uncertainty in the toxicity values is included. Here, the toxicity value and the degradation rate would therefore be the first to receive in-depth attention.

Table 6 Sensitivity table for calculation C: surface water with and without uncertain toxicity

	Parameters	**RCR Daphnia 0 days** With uncertainty in LC50	**RCR Daphnia 0 days** Without uncertainty in LC50
	$DT50_{water}$	49.9	99.0
	$LC50_{Daphnia}$	49.4	0.0
	VP	0.4	0.1
	Kow	0.0	0.2
	$DT50_{soil}$	0.0	0.1
*	SOL	0.2	0.2
*	Kom	0.1	0.3

* Correlated assumption

Deterministic RCR values were similar to the 50 percentile values of the distribution, or the median risk level (Table 7). Similar to calculation A, risk levels were again higher if calculated with USES 3.0, compared to USES 1.0.

Table 7 Results of the deterministic and probabilistic approach for calculation C: surface water with and without uncertain toxicity. See also explanation in Table 3.

	Daphnia With uncertainty in LC50	**Daphnia** Without uncertainty in LC50
Deterministic		
USES 1.0 log RCR	-4.30	-4.30
USES 3.0 log RCR	-4.16	-4.16
Probabilistic		
50 % log RCR	-4.16	-4.16
90 % log RCR	-4.14	-4.15
95 % log RCR	-4.13	-4.15
USES 1.0 percentile	2.5	2.5
USES 3.0 percentile	50.0	50.0

D. Target soil with uncertain toxicity

When the toxicity (LC50) for Eisenia was added to the uncertain parameters, again, uncertainty in the risk quotient increased (Figure 7) and the distribution becomes more sigmoidal. Based on the risks of the earthworm (Eisenia), the pesticide can be registered if it complies with the following criteria according to the Manual for the Registration of Pesticides (CTB, 1999):

- It is out of the question that the substance will end up on the soil surface;
- The PEC0/LC50 < 0.001;
- 0.001 ≤ PEC0/LC50 < 0.1, the DT90 < 100 days and there are ≤ 3 applications per season;
- 0.001 ≤ PEC0/LC50 < 0.1 and the PEC/NOEC < 0.2.

The complete distribution for the end point earthworm lies between the limits of an RCR (PEC0/LC50) of 0.001 and 0.1 (log RCR of –3 and –1, respectively). For this pesticide the DT90 is higher than 100 days and therefore a NOEC must become available, to check if this pesticide complies with the PEC/NOEC < 0.2 criterion (CTB, 1999). An adequate NOEC was not present in the risk assessment report for registration. Therefore, a supplemental chronic toxicity data was thought to be necessary. With that data, a new cumulative probability distribution plot can be made to determine the position of the distribution compared to following criterion for registration (CTB, 1999), the RCR (PEC/NOEC) of 0.2 (log RCR of –0.70).

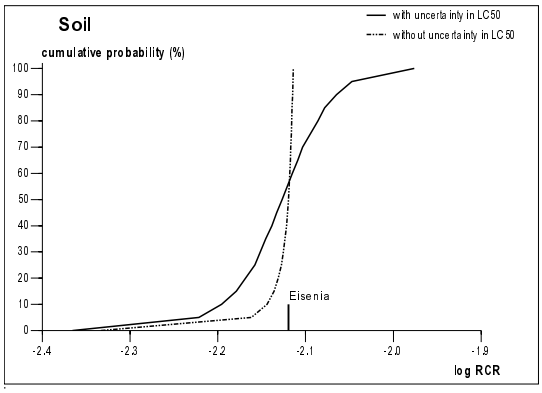


Figure 7 Cumulative probability distribution for the risk quotient of earthworm (Eisenia) with and without uncertainty in the LC50. The deterministic RCR value for this end point that was calculated with the quotient approach (USES 3.0) is indicated with a short vertical bar on the x-axis.

The $LC50_{Eisenia}$ contributed most to the uncertainty in RCR, when uncertainty in LC50 is taken into account (Table 8). However, without uncertainty in LC50, $DT50_{soil}$ was the most important parameter. Here, the toxicity value would be the first to receive in-depth attention.

Table 8 Sensitivity table for calculation D: target soil with and without uncertain toxicity.

Parameters	**RCR Eisenia 0 days** With uncertainty in LC50	**RCR Eisenia 0 days** Without uncertainty in LC50
$LC50_{Eisenia}$	89.5	0.0
$DT50_{soil}$	9.6	99.4
Kow	0.0	0.0
SOL	0.0	0.1
VP	0.6	0.3
$DT50_{water}$	0.0	0.1
Kom	0.2	0.1

Deterministic RCR values were similar to the 50 percentile values of the distribution, or the median risk level (Table 9). Risk levels were lower this time, when calculated with USES 3.0 compared to USES 1.0.

Table 9 Results of the deterministic and probabilistic approach for calculation D: target soil with and without uncertain toxicity. See also explanation in Table 3.

	Eisenia With uncertainty in LC50	**Eisenia** Without uncertainty in LC50
Deterministic		
USES 1.0 log RCR	-2.03	-2.03
USES 3.0 log RCR	-2.12	-2.12
Probabilistic		
50 % log RCR	-2.13	-2.12
90 % log RCR	-2.06	-2.11
95 % log RCR	-2.05	-2.11
USES 1.0 percentile	95.0	100.0
USES 3.0 percentile	55.0	50.0

6.2 Approach 2

For five additional pesticides, a probabilistic exposure assessment is executed. This assessment is based on data from the database of Mackay (1999). Three examples of calculations are carried out:

E. Uncertainty in concentration in **surface water (ditch)** is calculated.
   Concentration in water after 21 days is used to describe differences in pesticides.
F. Uncertainty in concentration in **target soil** is calculated.
   Concentration in soil after 0 days is used to describe differences in pesticides.
G. Uncertainty in concentration in **groundwater** is calculated.
   This calculation describes the leaching of a pesticide to groundwater.

Specifications of the example pesticide and the five other pesticides are listed in Table 10. Pesticides were selected on the basis of a wide range of input-parameter values, to see whether the previous results of the example pesticide were exceptional or not.

Table 10 Summary of the input parameter values (mean, k-factor) for several pesticides.

Pesticides	Log Kow (-)		VP (Pa)		SOL (mg/l)		Koc (l/kg)		$DT50_{water}$ (d)		$DT50_{soil}$ (d)	
	mean	k	Mean	k	Mean	k	mean	k	mean	k	mean	k
Example	0.55	4.3	2.0E-7	6.8	495.0	1.8	153	5.1	113.0	17.1	180.0	8.5
1.	2.96	4.3	3.3E-3	6.8	199.5	1.8	155	5.1	72.4	17.1	18.2	8.5
2.	3.95	30.2	3.9E-3	6.8	12.8	8.7	1677	5.1	59.4	17.1	5.8	8.5
3.	3.58	30.2	7.5E-4	6.8	0.3	8.7	6529	5.1	7.6	17.1	14.9	8.5
4.	4.69	30.2	1.5E-3	6.8	0.1	8.7	81521	5.1	784.0	17.1	663.0	8.5
5.	4.87	30.2	1.5E-2	3.0	1.0	8.7	8262	5.1	0.04	17.1	52.8	8.5

E. Surface water (ditch)

The cumulative probability of the concentration in surface water after 21 days differed substantially between pesticides (Figure 8). The distribution of the example pesticide was at the edge of all possible types of distributions and appeared to be rather an exceptional case than a general one. The slope of the graph is an indication for the uncertainty. For surface water, the uncertainty in the results of pesticides A and B is lower than for pesticides C and D (Figure 8). For pesticides with a steep slope, the uncertainty in the result is low. The right-hand tail is missing for pesticides A, B and example. This is again, probably due to the fact that the end of the TOXSWA table is reached. Values for $DT50_{water}$ beyond 1000 days are not included in this table. With an uncertainty factor of 17.1 (Table 2) and a mean $DT50_{water}$ of more than 60 days (Table 10), it is not unlikely that the end of the TOXSWA table will be reached. Therefore, RCR values at the right side of the sigmoid are missing. Pesticide D has a high $DT50_{water}$ value also, but for this pesticide, the $DT50_{water}$ is not contributing to the uncertainty in the concentration in surface water after 21 days.

For all example pesticides, the same maximum value of the concentrations in surface water can be observed in Figure 8. This is probably due to the fact that at that point the end of the TOXSWA table is reached. For the example pesticide, the risk limit is exceeded if the $PEC_{21\ days}$/NOEC for Daphnia is larger than 0.1 (CTB, 1999). With the NOEC for Daphnia of 1.8 mg/l a critical $PEC_{21\ days}$ of 180 μg/l can be calculated. According to the 'Decree Environmental demands for the registration of Pesticides' (BMB, 1995), an adequate risk evaluation is not

required, because the complete distribution of the example pesticide is below the value of 180 µg/l (log $PEC_{21\ days}$ = -0.75).

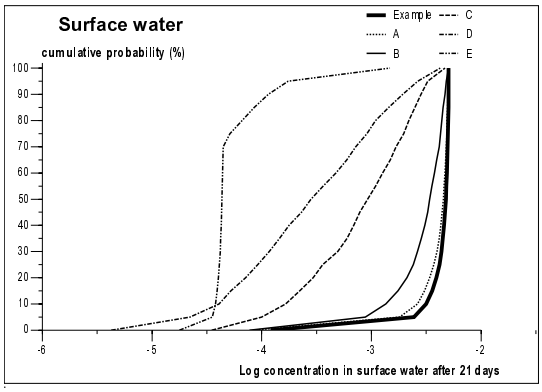


Figure 8 Cumulative probability distributions for the example pesticide and five additional pesticides in surface water.

The main sources of uncertainty can be selected from Table 11. For the example pesticide, $DT50_{water}$ is the most important input parameter, whereas for most of the other pesticides Kom, vapour pressure and solubility are more important. Only for pesticide D the degradation is not a sensitive parameter and therefore the uncertainty in the results can only decrease with more accurate data for solubility, vapour pressure and Kom. The correlation of solubility and Kow was not taken into account, because Kow is not contributing to the uncertainty of the endpoint. Kom, which is entered directly and which is not derived from Kow, is correlated to SOL instead.

Table 11 Sensitivity table for calculation E: surface water without toxicity

	Parameters	Example	A	B	C	D	E
	$DT50_{water}$	99.7	98.1	42.3	31.8	0.0	38.3
	Kow	0.0	0.0	0.0	0.2	0.0	0.4
*	Kom	0.1	0.3	15.7	18.0	27.0	35.5
	VP	0.2	0.9	17.7	23.1	30.5	1.5
*	SOL	0.0	0.7	24.3	27.0	42.4	24.2
	$DT50_{soil}$	0.0	0.0	0.1	0.0	0.1	0.1

* Correlated assumption

The deterministic surface water concentration is mostly around the 50 percentile values of the distributions (Table 12). The example pesticide has the highest surface water concentration after 21 days, probably due to an extremely low Kow value, high solubility and low vapour pressure.

Table 12 Results of the deterministic and probabilistic approach for calculation E: surface water without toxicity

	Example	A	B	C	D	E
Deterministic						
USES 3.0 log conc.	-2.32	-2.34	-2.41	-2.85	-3.50	-4.37
Probabilistic						
50 % log conc.	-2.32	-2.34	-2.47	-3.04	-3.55	-4.36
90 % log conc.	-2.30	-2.30	-2.33	-2.55	-2.71	-3.94
95 % log conc.	-2.30	-2.30	-2.32	-2.49	-2.58	-3.76
USES 3.0 percentile	50	50	65	65	52	40

F. Target soil

The example pesticide has a relatively high concentration in soil, which is higher than for most other pesticides (Figure 9). Here, only substance D has a higher concentration in soil after 0 days than the example pesticide. From Figure 9 it can be read that, for all pesticides, the concentration in soil is not higher than 0.1 mg/kg (or log concentration of –1.0). This is the result of the following calculation method of the concentration in soil (RIVM, VROM, VWS, 1999):

$$F_{rs} = e^{-kdeg_{soil} \cdot T_{interval}} \quad (1)$$

$$Csoil_{pest-0} = Csoil_{pest-1\,appl} \cdot \frac{1 - F_{rs}^{N_{appl}}}{1 - F_{rs}} \quad (2)$$

with N_{appl} = 2 this equation 2 can be rewritten:

$$Csoil_{pest-0} = Csoil_{pest-1\,appl} \cdot \frac{(1 + F_{rs}) \cdot (1 - F_{rs})}{1 - F_{rs}} \quad (3)$$

Input

F_{rs}	fraction of the concentration remaining in soil after time $T_{interval}$	[-]
$kdeg_{soil}$	rate constant for degradation in soil	[d^{-1}]
$T_{interval}$	application interval	[d]
$Csoil_{pest-1\,appl}$	concentration in soil after one application	[$kg_c.kg_{wwt}^{-1}$]
N_{appl}	number of applications in one year (equals 2 in this scenario)	[-]
Output		
$Csoil_{pest-0}$	peak concentration in soil after *N* applications	[$kg_c.kg_{wwt}^{-1}$]

Since $DT50_{soil}$ (=ln2/$kdeg_{soil}$) is the only input parameter that contributes to the uncertainty of the end-point, F_{rs} is the only factor in the calculation that has an uncertainty. According to the equations above, F_{rs} may vary between 0 and 1 (equation 1). Therefore, $Csoil_{pest-1appl}$ is multiplied with a factor between 1 and 2 (equation 3). Since the same scenario and the same dose was used for all pesticides, the minimum and maximum value of the endpoints are equal too. Based on the risk for earthworm a pesticide can be registered if the PEC0/LC50 is smaller than 0.001 (CTB, 1999). With this information, a critical LC50 for earthworm of 100 mg/kg can be calculated. Depending on the uncertainty in the LC50, the risk for earthworm is low if the LC50 is higher than 100 mg/kg.

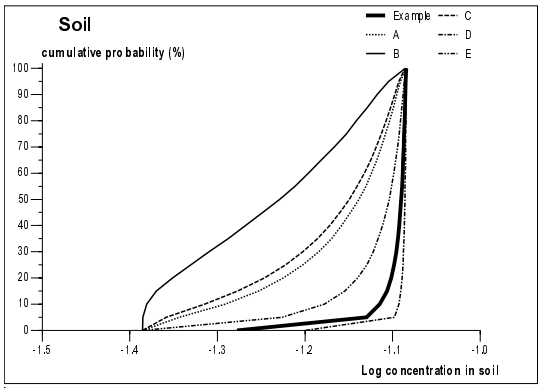


Figure 9 Cumulative probability distributions for the example pesticide and five additional pesticides in soil.

$DT50_{soil}$ is for all examined pesticides the most important parameter (Table 13). It is responsible for most of the uncertainty in soil concentration.

Table 13 Sensitivity table for calculation F: target soil without toxicity.

Parameters	Example	A	B	C	D	E
$DT50_{soil}$	99.8	98.9	99.7	98.9	99.3	98.3
VP	0.0	0.0	0.0	0.1	0.1	0.3
Kow	0.0	0.6	0.3	0.0	0.0	0.1
Kom	0.0	0.0	0.0	0.1	0.1	1.2
SOL	0.0	0.4	0.0	0.8	0.4	0.1
$DT50_{water}$	0.2	0.0	0.0	0.1	0.0	0.0

The deterministic soil concentration is similar to the 50-percentile value of the distributions (Table 14). The example pesticide and substance D have the highest soil concentration after 0 days, probably due to a relatively high $DT50_{soil}$ value.

Table 14 Results of the deterministic and probabilistic approach for calculation F: target soil without toxicity.

	Example	A	B	C	D	E
Deterministic						
USES 3.0 log conc.	-1.09	-1.14	-1.23	-1.15	-1.09	-1.10
Probabilistic						
50 % log conc.	-1.09	-1.14	-1.23	-1.15	-1.09	-1.10
90 % log conc.	-1.09	-1.10	-1.12	-1.10	-1.08	-1.09
95 % log conc.	-1.09	-1.09	-1.10	-1.09	-1.08	-1.09
USES 3.0 percentile	50	50	50	50	50	50

G. Groundwater

The cumulative probability of the concentration in groundwater differed substantially between pesticides (Figure 10). The distribution of the example pesticide was again at the edge of all possible types of distributions and appeared to be rather an exceptional response than a general one. The relevant admission criterion concerns the leaching of a pesticide to groundwater. A pesticide can be registered if the concentration < 0.000001 mg/l (log value = -6) and cannot be registered if the concentration > 0.001 mg/l (log value = -3) (CTB, 1999). Here, these limit values are based on a criterion of 0.0001 mg/l (log value = -4), for which an uncertainty factor of 100 is assumed. This additional uncertainty factor has been incorporated as an admission criterion, and is based on:

- Model uncertainty;
- Scenario uncertainty;
- Uncertainty in the DT50 and Kom, because a small spread in the DT50 and Kom resulted in a large spread of the model results.

This calculation only accounts for the last mentioned uncertainty and therefore could not explain the use and the size of the uncertainty factor of 100. Hence, only the uncertainty in DT50 and Kom and is compared with the limit value of 0.0001 mg/l (log value = -4), to determine the registration of the pesticide. For the example pesticide and pesticide D, about 75% and 60% of the distribution is above the critical concentration below which a pesticide can be registered. Most likely for both pesticides an additional leaching study is needed to determine the actual risk. Nevertheless, it is up to the decision-maker what percentile is an acceptable risk for leaching to groundwater. Compared to the deterministic result it can be better judged how much the RCR must change to obtain an acceptable risk estimate.

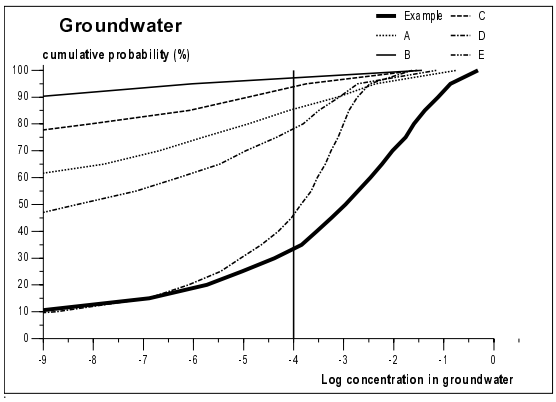


Figure 10 Cumulative probability distributions for the example pesticide and five additional pesticides in groundwater. The large vertical bar is an indication for the registration of a pesticide. At a concentration < 0.0001 mg/l (log value = -4) the risk for leaching to groundwater is low.

$DT50_{soil}$ is for all examined pesticides the most important parameter (Table 15). Only for the example pesticide and pesticide A the Kom is also relatively important. It is remarkable that for the example pesticides the results are more sensitive for the sorption (Kom) than for the degradation in soil (Table 15).

Table 15 Sensitivity table for calculation G: groundwater without toxicity.

Parameters	Example	A	B	C	D	E
Kom	46.6	30.1	4.4	2.0	8.9	8.5
$DT50_{soil}$	53.2	68.3	93.9	95.8	90.2	90.6
Kow	0.1	0.3	0.1	0.3	0.0	0.3
SOL	0.0	1.2	1.5	1.5	0.7	0.1
$DT50_{water}$	0.1	0.1	0.1	0.5	0.1	0.0
VP	0.0	0.0	0.0	0.0	0.0	0.4

Compared to the results of the risk assessment for registration, the results of the uncertainty analysis with USES 3.0 are more conservative for the example pesticide. With USES 1.0, a log concentration in groundwater of -3.3 was calculated compared to a log concentration of –2.6 for USES 3.0 (Table 16).

The deterministic groundwater concentration is similar to the 50-percentile value of the distributions (Table 16). The example pesticide and substance D have the highest groundwater concentration, probably due to a relatively high DT50 for soil.

Table 16 Results of the deterministic and probabilistic approach for calculation G: groundwater without toxicity

	Example	A	B	C	D	E
Deterministic						
USES 1.0 log conc.	-3.3	n.a.	n.a.	n.a.	n.a.	n.a.
USES 3.0 log conc.	-2.6	< -9.0	< -9.0	< -9.0	-3.9	-8.4
Probabilistic						
50 % log conc.	-3.0	< -9.0	< -9.0	< -9.0	-3.9	-8.3
90 % log conc.	-1.1	-3.1	-9.0	-4.9	-2.7	-3.1
95 % log conc.	-0.9	-2.4	-6.0	-3.7	-2.5	-2.7
USES 3.0 percentile	60	n.a.	n.a.	n.a.	50	50

n.a. not available

7. Conclusion

Decision-makers working in the framework of legalisation of pesticides rely on point estimates and do not account explicitly, neither qualitatively nor quantitatively, for the uncertainty in the assessment. Risk assessors use reasonable worst-case assumptions as a common approach for dealing with uncertainties associated with the methodology of assessing pesticides. It is claimed that this approach prevents an underestimation of the calculated risks. However, may lead to unrealistic assessments. This report tries to demonstrate that uncertainty analysis can improve risk assessment and the decision-making process. The decision-maker at least needs to understand which uncertainties are incorporated in the assessment and which not. Therefore, the uncertainties in the risk assessment should be taken into account in a transparent way to facilitate the interpretation of the results of an assessment. A probabilistic risk assessment can provide decision-makers with a better knowledge about the uncertainties to be taken into account in risk management decisions. Therefore, more attention is given to the probabilistic risk assessment of pesticides in the main international frameworks. This topic is mentioned in guidance documents and proposals are presented to reduce uncertainties. Nevertheless, in none of the international frameworks concerning the assessment of pesticides, an actual probabilistic analysis has been carried out or is incorporated in the different models or programs (see Chapter 3). Based on studies on new and existing chemicals, the advantages and disadvantages of the deterministic and probabilistic approach are summarised in Table 17 (Jager et al., 1997). This table is completed with advantages and disadvantages resulting from the probabilistic assessment of agricultural pesticides.

Table 17 Summary of the advantages and disadvantages of a probabilistic risk assessment

	Advantage	Disadvantage
Deterministic approach	– Rapid – Criterion is easy to interpret for decision-makers – Well established	– Little information about the risk – Unknown degree of conservatism – The results suggests too high precision
Probabilistic approach	– Lot of information about the risk estimate – Better comparison between chemicals – Identifies main source(s) of uncertainty – Worst case assumptions can be avoided – Stimulates research that may reduce uncertainty	– Relatively time and computer resources consuming – Less easy to interpret (probability distribution) – Relatively complex subject for decision-makers – Difficulties in risk communication

For a probabilistic assessment, probability distributions must be defined for the input parameters, which is illustrated in Appendix 3. This is not a thorough worked out guideline, but must be seen as an example to approach the problem of defining distributions. To gain better insight into an uncertainty analysis, two examples of calculations are discussed: one example pesticide already assessed for registration (uncertain PEC, deterministic and uncertain toxicity) and a comparison between several pesticides (uncertain PEC). More details about the calculations are presented in Chapter 6.

Introduction of uncertainty in the chosen input parameters can be an improvement compared to the deterministic calculation. The degree of uncertainty can be identified, which can be of great value for further research. This can provide decision-makers with the parameters that would be the first to receive in-depth attention.

The probabilistic calculations have resulted in the following conclusions:
– From the shape and steepness of the probabilistic curve it can be better judged how much the deterministic criterion must change to obtain an acceptable risk estimate;
– Uncertainties in the results of USES depend on the (uncertainties and variabilities of the) properties of the chemical;
– A more realistic assessment is possible when uncertainty in toxicity is incorporated;
– Introduction of uncertainty can be an improvement compared to the deterministic calculation, because a better comparison between pesticides is possible (factors contributing most to the uncertainty will be indicated and this may improve priority setting);
– For each pesticide, different input parameters may dominate the uncertainty in the results;
– It is possible to characterise the differences between subsequent model versions of USES in a better way;
– The shape of the curve of the cumulative probability plot can be an indication for the limitations of the model or model input (too much uncertainty in the extreme values in the models TOXSWA and PEARL).

The registration of pesticides is directly influenced by a probabilistic analysis. The Manual for the Registration of Pesticides (CTB, 1999) presents background information about the factors by which the risk limits for the leaching to groundwater and for surface water organisms can be exceeded.
For the risk limit for leaching to groundwater an additional uncertainty factor of 100 is incorporated, based on the fact that a small spread in the DT50 and Kom resulted in a large spread in the results of the model. With a probabilistic analysis this additional factor 100 may be reduced when uncertainty is incorporated in the distributions of the DT50 and Kom. Calculation G (Section 6.2) presents the probabilistic analysis for the leaching to groundwater, without using the uncertainty factor of 100.
In the Manual for the Registration of Pesticides a distinction is made between the calculated risk for surface water organisms that exceed the risk limit with less or more than a factor 100. This exceeding factor of 100 is used because of the accumulation of uncertainties in the calculations of the used models. For the example pesticide in this report, the risk limit for surface water was not exceeded and therefore the factor 100 could not be exemplified.
When an uncertainty analysis is used, the current additional uncertainty factors incorporated in the risk limits for the registration of pesticides may be reduced.

When the results are interpreted, it must be kept in mind that only chemical-specific uncertainties and variabilities were quantified and that important other sources of uncertainty and variability are ignored. The probabilistic risk assessment did not directly influence the conclusion of the registration of the example pesticide. The uncertainties in the results of USES depend on different chemical properties of a pesticide. Generally, the variability in degradation is the main source of uncertainty. Nevertheless, for the surface water end points of some example pesticides also Kom, VP and SOL are important. For groundwater, not only degradation but also Kom is a main source of uncertainty. Degradation becomes less important when uncertainty in the toxicity values is included. The uncertainty analysis of the effect assessment is only briefly discussed in this report. Nevertheless, recommendations are made for a better implementation of a probabilistic analysis in the effect assessment (see appendix 4). This report is meant and must be seen as a discussion document for decision-makers to become acquainted with probabilistic methods. More effort is needed before uncertainty analysis can be incorporated in the routine assessment of pesticides.

Discussion points

The examples of calculations show that decision-makers can be presented with more information to base their decisions on. Several questions must be answered, if we want to make the transition from deterministic to probabilistic risk assessments. The problem of uncertainty in risk assessment is relatively large and can quickly become too complex for decision-makers. Still, a solution must be found to manage this issue and to make the probabilistic assessments more consistent and easier to evaluate. To some extent this issue can be managed through standardisation of the probabilistic risk assessment of pesticides. For a clearer understanding it is advisable to describe which assessments need a probabilistic analysis and in which cases it is unnecessary. Guidance is available in for instance Roberts (1999), Warren-Hicks and Moore (1998), or EPA (1997). Another aspect of probabilistic assessments is that decision-makers have to adapt themselves to deal with a risk distribution rather than a single deterministic expression of the exposure or risk. If they want to use the results of probabilistic assessments they must determine the acceptability of the risk, in other words, at which percentile of the distribution is the risk characterisation ratio acceptable. With a probabilistic assessment, acceptable decisions will usually be made based on risks at defined percentiles. Furthermore, decision-makers also have to get used to communicate about probabilistic assessments with stakeholders, among others the general people. It is reasonable to expect that this will lead, in some cases, to more vigorous discussions between decision-makers and the public, industry and farmers regarding the meaning of a probabilistic assessment and reasonable levels of protection. This requires a well thought-out communication strategy to insure that discussions are productive.

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Appendix 1 Mailing list

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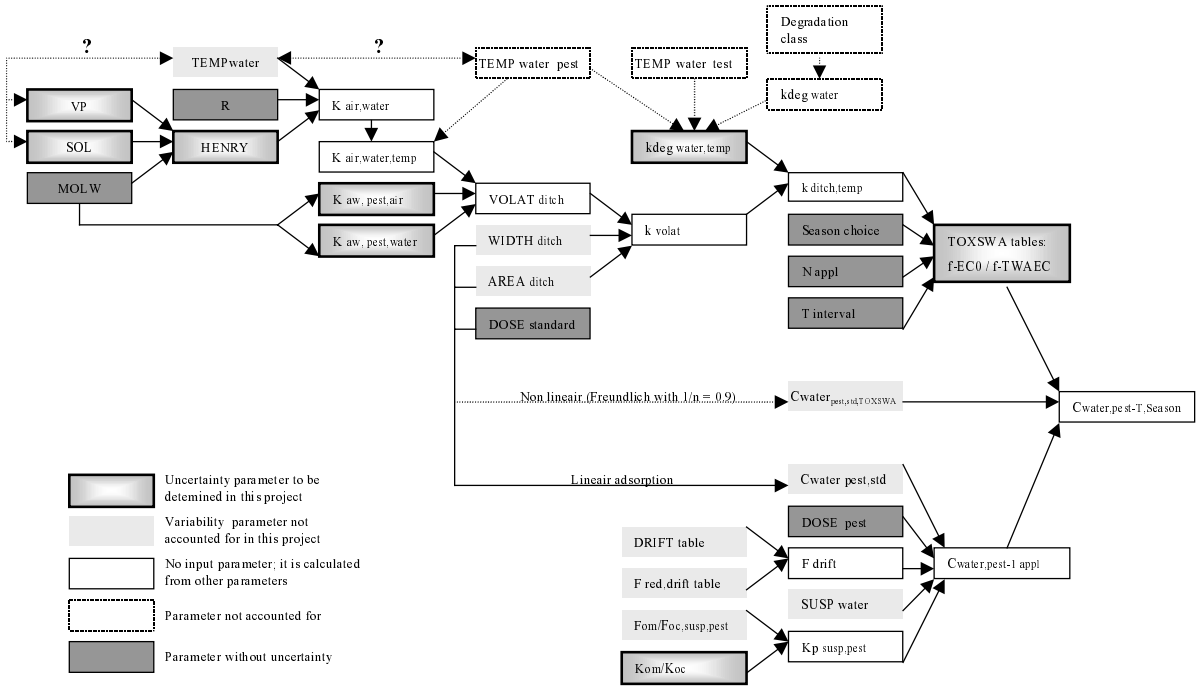
Appendix 2 Choice of uncertain parameters

A. Spray: concentration water ditch

Spray: concentration water ditch



U/V[2]	Symbol	Description	Unit	Flag[3]	Equation nr. [4]
Uncertainty parameters distribution determined in this report:					
U	VP	vapour pressure	[Pa]	S	22
U	SOL	water solubility	[$kg_c.m^{-3}$]	S	22
U	HENRY	Henry's law constant	[$Pa.m^3.mol^{-1}$]	O	23
U	$kdeg_{water,temp}$	temp dependent rate constant for degradation	[d^{-1}]	O	P-132
U	Koc	organic carbon-water partitioning coefficient	[$m^3.kg^{-1}$]	O	P-124A
U	Kom	organic matter-water partitioning coefficient	[$m^3.kg^{-1}$]	O	P-124B
U	TOXSWA Tables		[$\mu g.l^{-1}$]	O	Appendix VIII
U/V	$Kaw\text{-}pest_{water}$	partial mass transfer coeff at water side...	[$m.d^{-1}$]	O	P-129
U/V	$Kaw\text{-}pest_{air}$	partial mass transfer coeff at air side…	[$m.d^{-1}$]	O	P-129
Variability parameters distribution not determined in this report:					
V	$Cwater_{pest,std,TOXSWA}$	TOXSWA std conc resulting from std input according to Freundlich adsorption in equation P-125 (=EC0)	[$kg.m^{-3}$]	D	TOXSWA ($4.732.10^{-6}$)
V	$Cwater_{pest,std}$	total conc resulting from a std input of 1 $mg.m^{-2}$	[$kg.m^{-3}$]	D	P-125 ($4.76.10^{-6}$)
V	$Foc_{susp,pest}$	weight fraction of organic carbon in susp matter	[$kg.kg^{-1}$]	D	P-124A (0.0294)
V	$Fom_{susp,pest}$	weight fraction of organic matter in susp matter	[$kg.kg^{-1}$]	D	P-124B (0.050)
V	TEMPwater	default temperature of water compartment	[12°C]	P	23
V	$WIDTH_{ditch}$	width of water surface in ditch	[m]	D	P-130 (1)
V	$AREA_{ditch}$	cross section of water layer in ditch	[m]	D	P-130 (0.21)
V	$SUSP_{water}$	concentration suspended solids in ditch	[$kg_{solid}.m_{water}^{-3}$]	D	P-125 (0.015)
V	DRIFT Table	fraction drift	[-]	O	Table A-4
V	$Fred_{drift}$	fraction emission reduction for drift	[-]	O	Table A-5

[2] U: Uncertain parameter V: Variable parameter
[3] O: Output parameter D: Standard default parameter S: Input data set parameter P: Parameter from 'pick list'
[4] Equation number as mentioned in USES manual (RIVM, VROM, VWS, 1999); Between brackets: value of default

Parameters not accounted for, because $kdeg_{water,temp}$ is input:

Degradation class; result of screening test biodegradability		[-]	P	Table III-6 p. III-28
$kdeg_{water}$	temp dependent rate constant for degradation	[d^{-1}]	O	36
$TEMPwater_{pest}$	pesticide temperature of water compartment	[10°C]	P	P-125A
$TEMPwater_{test}$	temp of water comp under test conditions	[20 °C]	D	P-125A

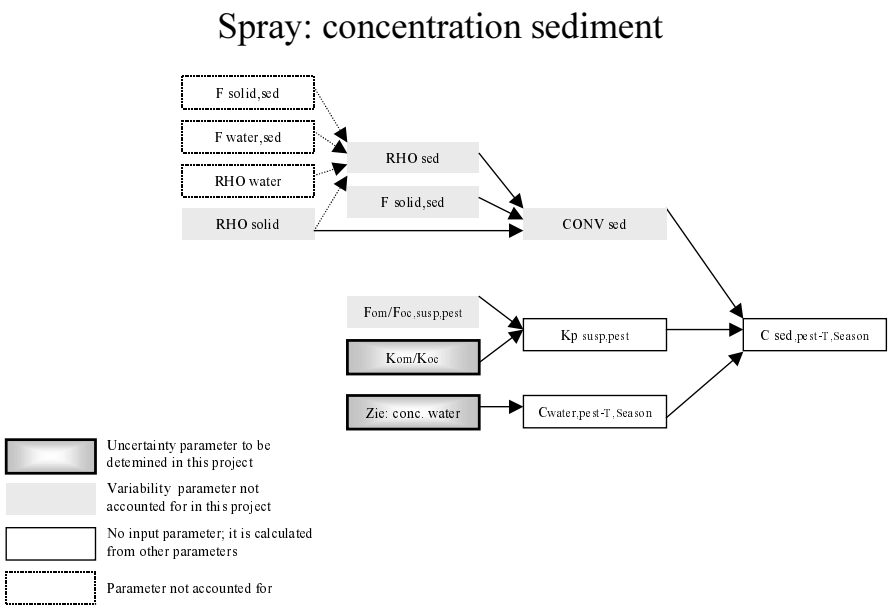
No parameter distribution (no uncertainty):

MOLW	molecular weight	[$kg_c.mol^{-1}$]	S	22
R	gas constant	[$Pa.m^3.mol^{-1}.K^{-1}$]	D	23 (8.314)
SeasonChoice	choice of season	[spring/autumn]	P	
$DOSE_{standard}$	standard dosage of pesticide = 1 $kg.m^{-2}$	[$kg.m^{-2}$]	D	P-124 C
N_{appl}	number of applications in one year	[-]	S	TOXSWA P-138
$T_{interval}$	application interval	[d]	S	TOXSWA
$DOSE_{pest}$	single dosage of pesticide	[$kg.m^{-2}$]	S	P-125

Parameter calculated according to equations with distribution included:

$K_{air\text{-}water}$	air-water partitioning coefficient	[$m^3.m^{-3}$]	O	23
$K_{air\text{-}water,temp}$	temperature corr air-water partitioning coefficient	[$m^3.m^{-3}$]	O	P-129
$VOLAT_{ditch}$	overall mass transfer coeff for volatilisation	[$m.d^{-1}$]	O	P-130
k_{volat}	first order rate constant for volatilisation in ditch	[d^{-1}]	O	P-132
$k_{ditch,temp}$	temp dependent total rate constant removal ditch	[d^{-1}]	O	P-132
F_{drift}	fraction drift related to location / way application	[-]	O	P-11
$Kp_{susp,pest}$	solids-water part coeff in susp matter	[$m^3.kg^{-1}$]	O	P-125
$Cwater_{pest,1appl}$	conc ditch after one application	[$kg.m^{-3}$]	O	P-125
$Cwater_{pest\text{-}T,Season}$	concentration in ditch over T days in season	[$kg.m^{-3}$]	O	not available

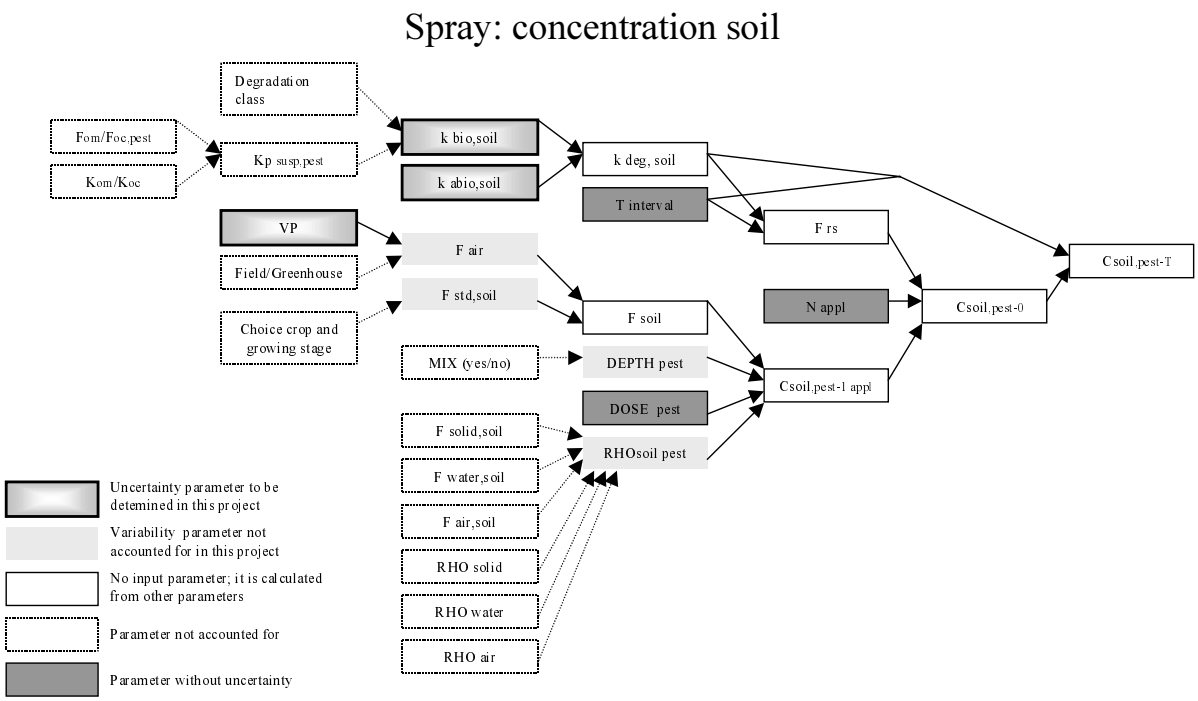
B. Spray: concentration sediment



U/V[5]	Symbol	Description	Unit	Flag[6]	Equation nr. [7]
Uncertainty parameters distribution to be determined in this report:					
U	Koc	organic carbon-water partitioning coefficient	[$m^3.kg^{-1}$]	O	P-124A
U	Kom	organic matter-water partitioning coefficient	[$m^3.kg^{-1}$]	O	P-124B
Variability parameters distribution not determined in this report:					
V	$Foc_{susp,pest}$	weight fraction of organic carbon in susp matter	[$kg.kg^{-1}$]	D	P-124A (0.0294)
V	$Fom_{susp,pest}$	weight fraction of organic matter in susp matter	[$kg.kg^{-1}$]	D	P-124B (0.050)
V	RHO_{sed}	wet bulk density of sediment	[$kg.m^{-3}$]	O	18
	Calculated with:				
	$Fwater_{sed}$	volume fraction of water in sediment	[$m^3.m^{-3}$]	D	15 (0.8)
	$Fsolid_{sed}$	volume fraction of solids in sediment	[$m^3.m^{-3}$]	D	15 (0.2)
	RHOwater	density of water phase	[$kg.m^{-3}$]	D	15 (1.0)
	RHOsolid	density of solid phase	[$kg.m^{-3}$]	D	15 (2.5)
V	$CONV_{sed}$	conversion factor for sediment conc: wwt to dwt	[$kg_{wwt}.kg_{dwt}^{-1}$]	O	18
	Calculated with:				
	RHO_{sed}	wet bulk density of sediment	[$kg.m^{-3}$]	O	18
	$Fsolid_{sed}$	volume fraction of solids in sediment	[$m^3.m^{-3}$]	D	15 (0.2)
	RHOsolid	density of solid phase	[$kg.m^{-3}$]	D	15 (2.5)
Parameter calculated according to equations with distribution included:					
$Kp_{susp,pest}$		solids-water part coeff in susp matter	[$m^3.kg^{-1}$]	O	P-125
$Cwater_{pest\text{-}T,Season}$		concentration in ditch over T days in season	[$kg.m^{-3}$]	O	TOXSWA
$Csed_{pest\text{-}T,Season}$		concentration in sediment over T days in season	[$kg.kg^{-1}$]	O	P-146

[5] U: Uncertain parameter V: Variable parameter
[6] O: Output parameter D: Standard default parameter S: Input data set parameter P: Parameter from 'pick list'
[7] Equation number as mentioned in USES manual (RIVM, VROM, VWS, 1999); Between brackets: value of default

C. Spray: concentration target soil



U/V[8]	Symbol	Description	Unit	Flag[9]	Equation nr. [10]	
Uncertainty parameters distribution to be determined in this report:						
U	VP	vapour pressure	[Pa]	S	22	
U	$kbio_{soil}$	rate constant for biodegradation in soil	[d^{-1}]	O	Table III-7	
U	$kabio_{soil}$	rate constant for abiotic degradation in soil	[d^{-1}]	D	Table III-4	(0)
Variability parameters distribution not determined in this report:						
V	$RHO_{soil, pest}$	bulk density of target soil	[$kg.m^{-3}$]	O	P-92	
	Calculated with:					
	$Fsolid_{soil}$	volume fraction of solids in soil	[$m^3.m^{-3}$]	D	14	
	$Fwater_{soil}$	volume fraction of water in soil	[$m^3.m^{-3}$]	D	14	
	$Fair_{soil}$	volume fraction of air in soil	[$m^3.m^{-3}$]	D	14	
	RHOsolid	density of solid phase	[$kg.m^{-3}$]	D	14	
	RHOwater	density of water phase	[$kg.m^{-3}$]	D	14	
	RHOair	density of air phase	[$kg.m^{-3}$]	D	14	
V	$DEPTH_{pest}$	mixing depth of target soil	[m]	O	P-92	
	Calculated with:					
	MIX	mixing with soil	[yes/no]	P		
V	F_{air}	fraction of dosage emitted to air	[-]	O	Table A-2	
	Calculated with:					
	Choice for field or greenhouse		[-]	P	Table A-2	
	VP	vapour pressure	[Pa]	S	22	
V	$Fstd_{soil}$	std fraction of dosage reaching soil, at 10% to air	[-]	O	Table A-3	
	Calculated with:					
	Choice of crop and growing stage		[-]	P	Table A-3	

[8] U: Uncertain parameter V: Variable parameter
[9] O: Output parameter D: Standard default parameter S: Input data set parameter P: Parameter from 'pick list'
[10] Equation number as mentioned in USES manual (RIVM, VROM, VWS, 1999); Between brackets: value of default

Parameters not accounted for, because $kbio_{soil}$ is input:

U	Koc	organic carbon-water partitioning coefficient	[$m^3.kg^{-1}$]	O	P-124A
U	Kom	organic matter-water partitioning coefficient	[$m^3.kg^{-1}$]	O	P-124B
U	$Kp_{susp,pest}$	solids-water part coeff in susp matter	[$m^3.kg^{-1}$]	O	P-125
U	Degradation class; result of screening test biodegradability		[-]	P	Table III-7 p. III-29
V	$Foc_{susp,pest}$	weight fraction of organic carbon in susp matter	[$kg.kg^{-1}$]	D	P-124A (0.0294)
V	$Fom_{susp,pest}$	weight fraction of organic matter in susp matter	[$kg.kg^{-1}$]	D	P-124B (0.050)

No parameter distribution (no uncertainty):

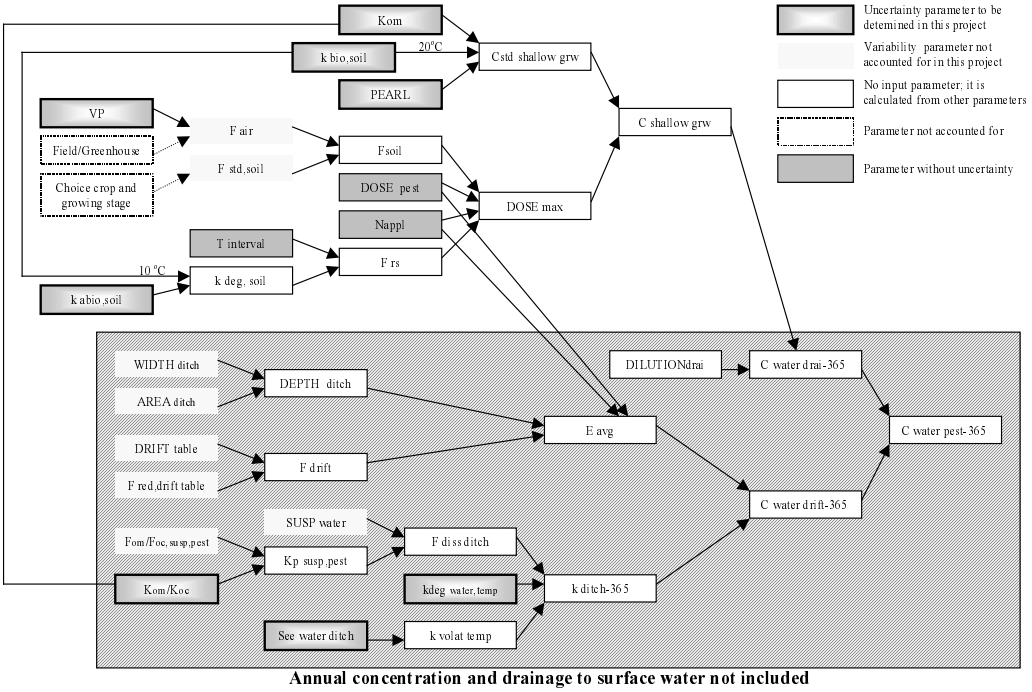
$T_{interval}$	application interval	[d]	S	P-93
N_{appl}	number of applications in one year	[-]	S	P-94
$DOSE_{pest}$	dosage	[$kg_c.m^{-2}$]	S	P-92

Parameter calculated according to equations with distribution included:

$kdeg_{soil}$	rate constant for degradation in soil	[d^{-1}]	O	P-93
F_{rs}	fraction of the concentration remaining after $T_{interval}$	[-]	O	P-94
F_{soil}	fraction of dosage that reaches the soil	[-]	O	P-92
$Csoil_{pest\text{-}1\,appl}$	concentration in soil after one application	[$kg_c.kg_{wwt}^{-1}$]	O	P-92
$Csoil_{pest\text{-}0}$	peak concentration in soil after N applications	[$kg_c.kg_{wwt}^{-1}$]	O	P-94
$Csoil_{pest\text{-}T}$	average soil concentration over T days	[$kg_c.kg_{wwt}^{-1}$]	O	P-95

D. Spray: concentration groundwater

Spray: concentration groundwater



Annual concentration and drainage to surface water not included

U/V[11]	Symbol	Description	Unit	Flag[12]	Equation nr. [13]

Uncertainty parameters distribution to be determined in this report:

U	VP	vapour pressure	[Pa]	S	22
U	Kom	organic matter-water partitioning coefficient	[$m^3.kg^{-1}$]	O	PEARL *III.4.9.5*
U	$Kbio_{soil}$	rate constant for biodegradation in soil	[d^{-1}]	O	PEARL Table III-7
U	$Kabio_{soil}$	rate constant for abiotic degradation in soil	[d^{-1}]	D	Table III-4 (0)
U	PEARL Tables (Kom and $DT50_{bio,soil}$ at 20°C)		[$ug.l^{-1}$]	O	Appendix VII

Variability parameters distribution not determined in this report:

V	F_{air}	fraction of dosage emitted to air	[-]	O	Table A-2
	Calculated with:				
	Choice for field or greenhouse		[-]	P	Table A-2
	VP	vapour pressure	[Pa]	S	22
V	$Fstd_{soil}$	std fraction of dosage reaching soil, at 10% to air	[-]	O	Table A-3
	Calculated with:				
Choice of crop and growing stage			[-]	P	Table A-3

No parameter distribution (no uncertainty):

$T_{interval}$	application interval	[d]	S	P-93
N_{appl}	number of applications in one year	[-]	S	P-94
$DOSE_{pest}$	dosage	[$kg_c.m^{-2}$]	S	P-92

Parameter calculated according to equations with distribution included:

$kdeg_{soil}$	rate constant for degradation in soil	[d^{-1}]	O	P-93
F_{rs}	fraction of the concentration remaining after $T_{interval}$	[-]	O	P-94
F_{soil}	fraction of dosage that reaches the soil	[-]	O	P-92
$DOSE_{max}$	apparent maximum dose	[$kg_c.m^{-2}$]	O	P-150A
$Cstd_{shallow\ grw}$	standard concentration in shallow groundwater	[($kg_c.m^{-3}$)/($kg_c.m^{-2}$)]	O	P-150A
$C_{shallow\ grw}$	concentration in shallow ground water	[$kg_c.m^{-3}$]	O	P-150A

[11] U: Uncertain parameter V: Variable parameter

[12] O: Output parameter D: Standard default parameter S: Input data set parameter P: Parameter from 'pick list'

[13] Equation number as mentioned in USES manual (RIVM, VROM, VWS, 1999); Between brackets: value of default value

Appendix 3 Parameter distributions

This appendix describes the derivation of the parameter distributions that were used for the examples of calculations. Several pesticides were selected, which showed a wide variety in their physico-chemical properties. Data were collected from literature sources (Mackay, 1999 and the ARS Pesticide Properties Database). Temperature corrections were done for Vapour Pressure (VP), Solubility (SOL) and Degradation in water ($DT50_{water}$) (Beltman and Adriaanse, 1999):

VPcorrected = VPt/(1*EXP((-95000/8.314)*((1/t)-(1/298))))
where t = temperature (Kelvin), and VPt = Vapour Pressure at temperature t.

SOLcorrected = SOLt/(1*EXP((-27000/8.314)*((1/t)-(1/298))))
where t = temperature (Kelvin), and SOLt = Solubility at temperature t.

$DT50_{water}$ corrected = $DT50_{water}$_t/(1*EXP(0.08*(298-t)))
where t = temperature (Kelvin), and $DT50_{water}$_t = Degradation at temperature t.

All the compounds used for the uncertainty analysis of each parameter are listed in Table A 1.

Table A 1 Compounds used for the derivation of probability distributions.

Name	CAS no.
Alachlor	15972-60-8
Aldicarb	116-06-3
Atrazine	1912-24-9
Azinphos-methyl	86-50-0
Carbaryl	63-25-2
Carbofuran	1563-66-2
Chlordane	57-74-9
Dichlorvos	62-73-7
Dimethoate	60-51-5
Disulfoton	298-04-4
Diuron	330-54-1
Endosulfan	115-29-7
Fenthion	55-38-9
Isofenphos	25311-71-1
Linuron	330-55-2
Methiocarb	2032-65-7
Metolachlor	51218-45-2
Metribuzin	21087-64-9
Oxamyl	25135-22-0
Phorate	298-02-2
Prometryn	7287-19-6
Propoxur	114-26-1
Quintozene	82-68-8
Simazine	122-34-9
Terbufos	13071-79-9
Terbutryn	886-50-0
Trichlorfon	52-68-6
Trifluralin	1582-09-8

Physico-chemical properties (Kow, SOL, VP, MOLW)

Uncertainty in the physico-chemical properties results from measurement errors, other measurement methods, etc. It may depend upon the absolute value of the parameter. For very hydrophobic chemicals, the uncertainty in *Kow* will be higher than for more hydrophilic chemicals. The uncertainty for poorly soluble chemicals will be higher than chemicals with a high solubility. Therefore, a different uncertainty is attached to different parts of the parameter range. The molecular weight is highly accurate and therefore the uncertainty is not relevant. The choice for cut-off values was mainly based on visual judgement from the residual plots of the log-linear regression against the geometric mean values of a parameter (Figures A1-A3). Reported k-values are the mean value of the k-values for the individual substances.

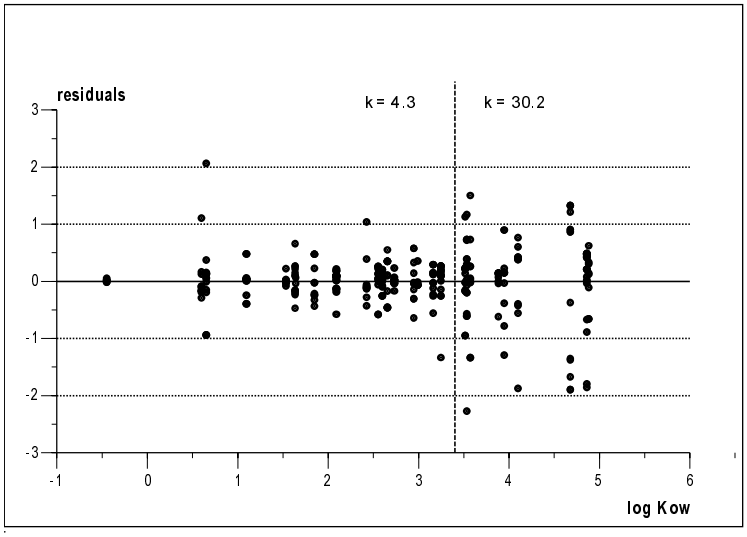


Figure A 1 ***Kow****: log Kow ≤ 3.4 (L; k=4.3) logKow >3.4 (L; k=30.2)*

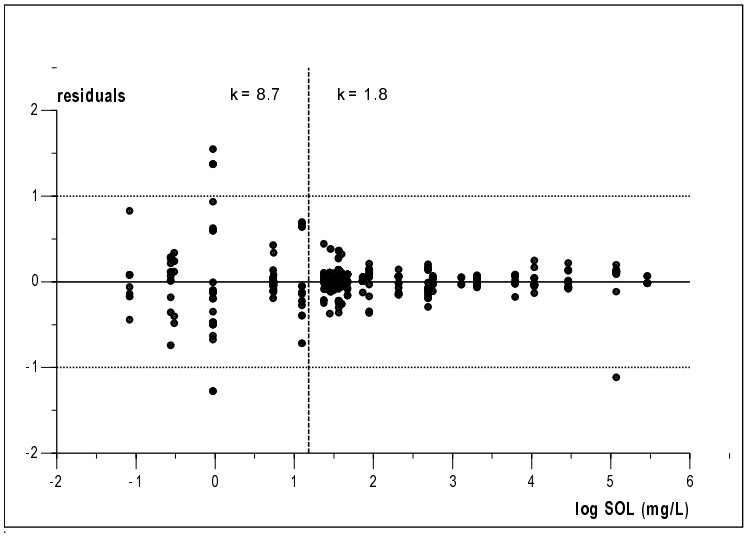


Figure A 2 ***Solubility****: SOL ≤ 15 mg/l (L; k=8.7) SOL >15 mg/l (L; k=1.8)*

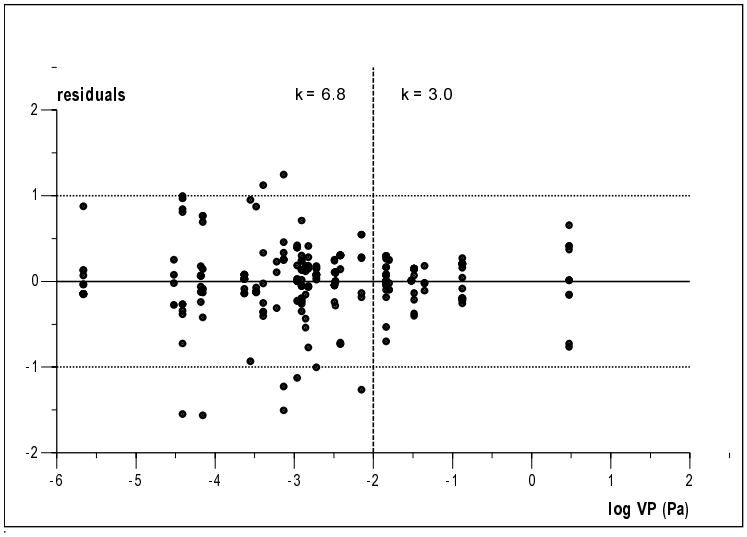


Figure A 3 ***Vapour pressure****: VP ≤ 0.01 Pa (L; k=6.8) VP > 0.01 Pa (L; k=3.0)*

The correlation between Kow and Koc, and between Kow and solubility were calculated from the average values on log scale (Figure A 4 and Figure A 5). These correlation coefficients are used in the sampling. The correlation coefficient between Kow and vapour pressure was not significant.

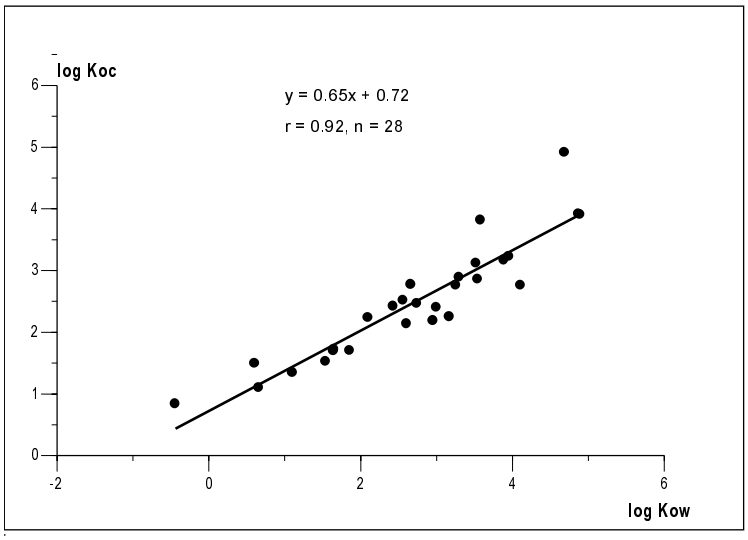


Figure A 4 Correlation between log Kow and log Koc (y=0.65x + 0.72)

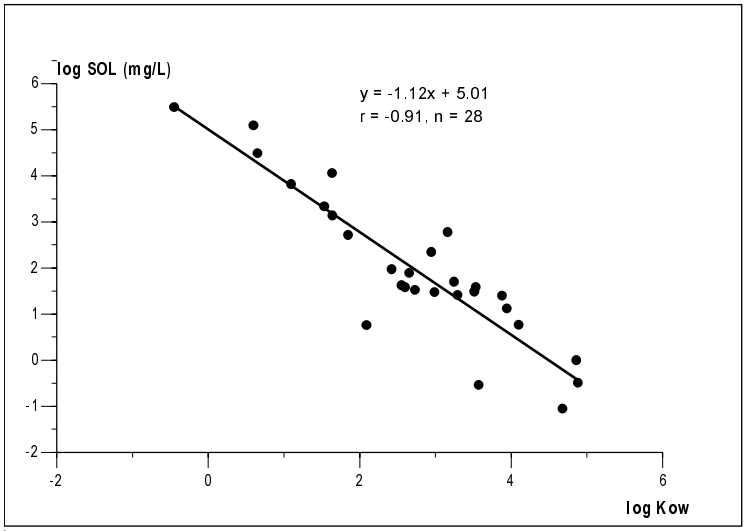


Figure A 5 Correlation between log Kow and solubility (y=-1.12x + 5.01)

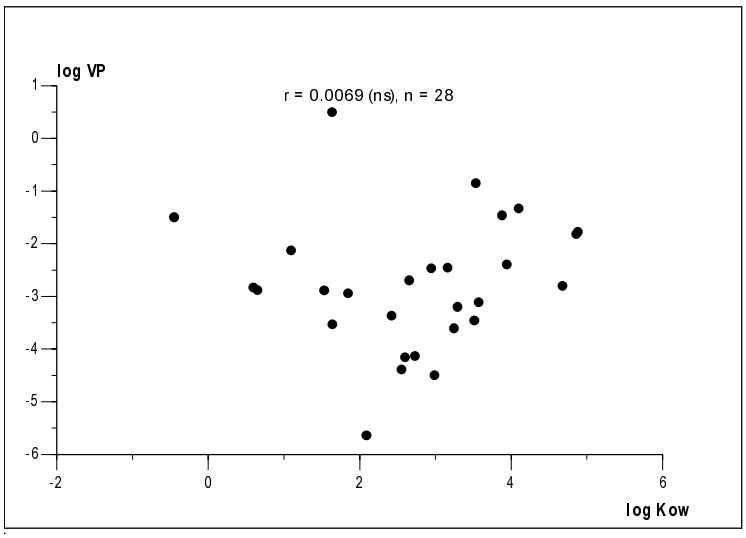


Figure A 6 Correlation between log Kow and vapour pressure

Partitioning coefficients (Kom, Koc, HENRY)

Uncertainty in Kom or Koc is mainly attributable to variability in soils; uncertainty in measurements usually contributes only slightly to the uncertainty. For the assessment of pesticides the Kom or Koc is a direct input for the USES 3.0 model and is not estimated from a Kow. The Kom and Koc are related to each other according to: Kom=Koc / 1.7. Because of this relation only the distribution for the Koc is determined. The Henry's law constant is generally calculated from the vapour pressure and the solubility. No additional uncertainty for this parameter is assumed. Only when a measured value is given for the Henry's law constant, an uncertainty needs to be attached to this parameter.

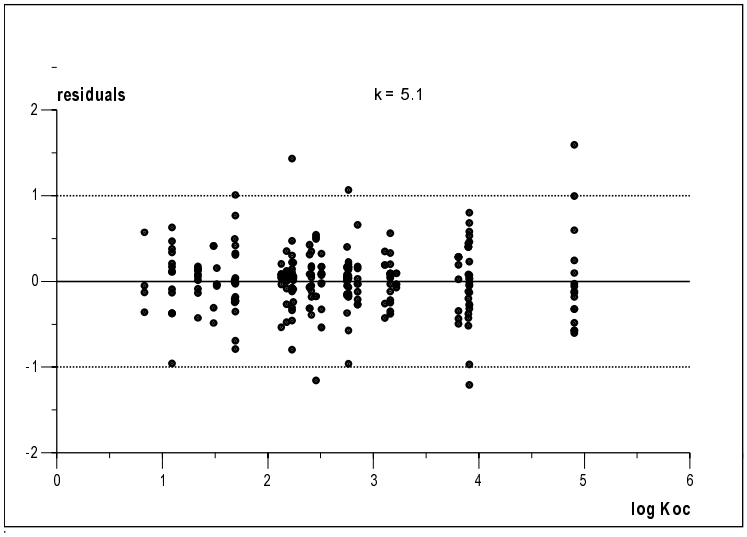


Figure A 7 ***Organic carbon normalised partitioning coefficient:*** *Koc (L; k=5.1)*

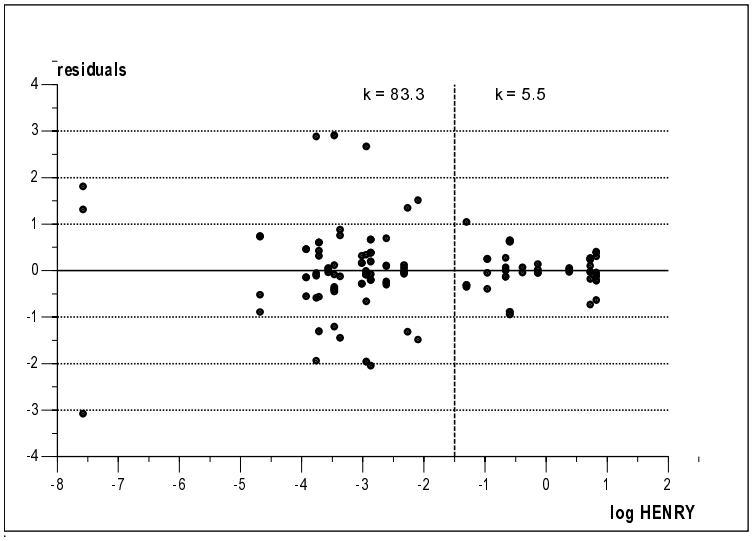


Figure A 8 ***Henry's law constant:*** *HENRY ≤ 0.03 (L; k=83.3) HENRY > 0.03 (L; k=5.5)*

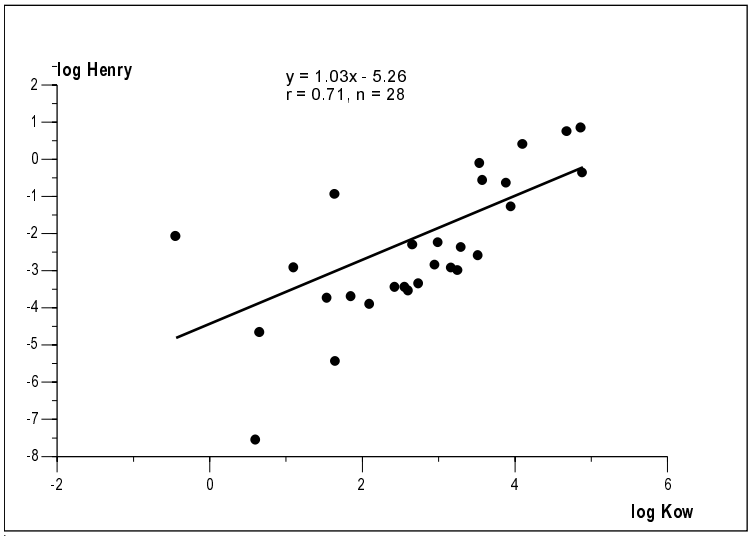


Figure A 9 Correlation between log Kow and Henry's law constant (y=-1.03x + 5.26)

Degradation ($DT50_{water}$, $DT50_{soil}$)

Uncertainty in $DT50_{water}$ and $DT50_{soil}$ is mainly attributable to variability in (natural) waters and soils; uncertainty in measurements usually contributes only slightly to the uncertainty. For the assessment of pesticides the degradation rates are a direct input for the USES 3.0 model and are not calculated from results of screening tests for biodegradability. The biodegradation depends on the temperature of the environment. The uncertainty in the temperature dependency is much lower than the uncertainty in the biodegradation. Therefore, the differences between the temperature of the modelled environment in USES 3.0 and the temperature under test conditions are not taken into account. The degradation can also depend on the concentration of the substance, but this effect is also not taken into account. The distributions are calculated from reported data in the literature.

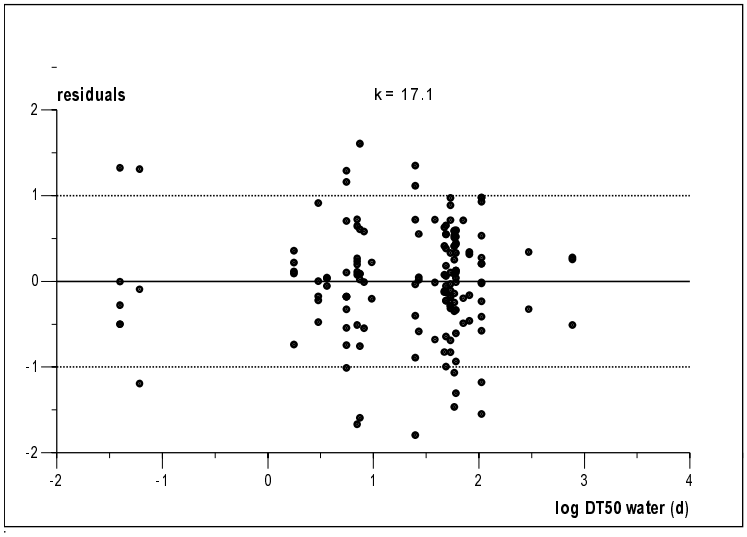


Figure A 10 ***Biodegradation in water****: $DT50_{water}$ (L; k=17.1)*

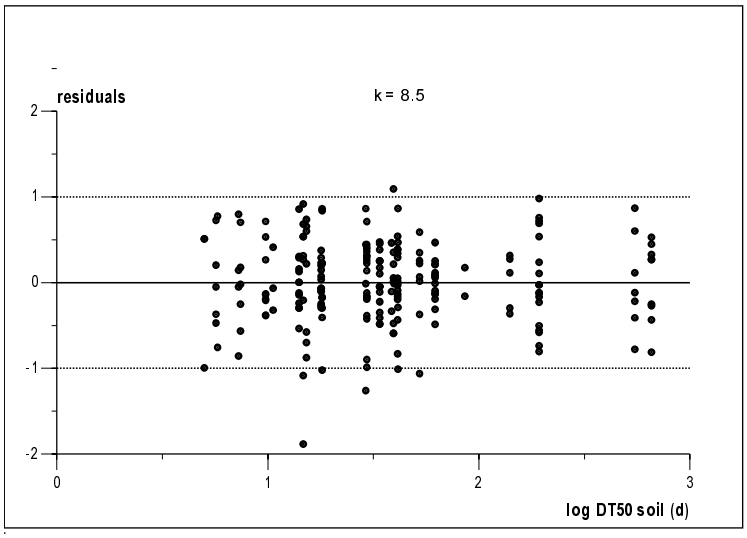


Figure A 11 ***Biodegradation in soil****: $DT50_{soil}$ (L; k=8.5)*

Single dosage of a pesticide, number of applications in one year and application interval (DOSE pest, N_{appl}, $T_{interval}$)

The single dosage of a pesticide, the number of applications in one year and the application interval are all uncertainty parameters. According to 'good agricultural practice' these parameters can assume to be deterministic and are therefore not accounted for in the probabilistic uncertainty assessments of this report.

Partial mass-transfer coefficients (Kaw-pest, water; Kaw-pest, air)

The partial mass-transfer coefficients depend on substance properties, but are not very uncertain. Wind, waves, bubbles and heat transfer have the greatest influence on k_w (4.8 m/d = 20 cm/h) and k_a (720 m/d = 3000 cm/h), which are all variables of the scenario (see RIVM, VROM, VWS, 1999; equations P-126 and P-127). The uncertainty caused by chemical properties or chemical reaction (of CO_2 and H_2O) is not more than 2-3 % (Liss and Slinn, 1983). Therefore, the uncertainty for the partial mass transfer coefficients is not taken into account.

TOXSWA and PEARL tables

The TOXSWA tables are based on a standard scenario and depend on the DT50 for water. Only the distribution of the DT50 for water is used to account for uncertainty related to TOXSWA. The DT50 of the water sediment system is not the same as the DT50 for water. Actually the latter must be the input for the TOXSWA tables. This form of 'imperfect data' is not taken into account.

The PEARL tables are also based on a standard scenario and depend on the Kom and the biodegradation in soil. Only the distribution of the Kom and the DT50 for soil is used to account for uncertainty related to PEARL.

Appendix 4 Procedure for implementation of uncertainty analysis in the effect assessment

In the risk assessment for plant protection products, toxicity data are generally not extrapolated to other species or to ecosystems. Instead, the resulting measure of toxicity (e.g., LC50, EC50, NOEC) is used in conjunction with the PEC to infer about the risk. In this way, only the summary statistic of the toxicity test results is used, ignoring other information contained in the data (e.g., slope of the dose-response relationship). Uncertainty analysis for the effects assessment usually looks at uncertainty in the LC50 (this report) or in the assessment factors (Roelofs, 2001).

There is however an alternative procedure possible, analogous to the use of species-sensitivity distributions to derive PNECs for ecosystems (Aldenberg and Slob, 1993). In this approach, a continuous function (e.g. log logistic or log normal) is fitted to the available toxicity data (usually NOECs) and the concentration is calculated at which 95% of the species is exposed below their NOEC. This procedure can also be reversed to yield the fraction of species affected at a given environmental concentration (Klepper et al., 1998), and uncertainty in this fraction can be calculated (Aldenberg and Jaworska, 2000).

In a similar way, the dose-response results for a single species (as given in the dossier) can be used to predict the fraction of the population of the species that is affected at a certain environmental concentration. Using the methodology outlined earlier (Aldenberg and Jaworska, 2000), the uncertainty in this fraction can be calculated. Furthermore, when an uncertain estimate of the PEC is available, these sources of uncertainty can be combined. An example of this procedure is shown in Figure A 12. The left panel shows the toxicity data obtained from the notifier. This dose-response relationship, with its uncertainty, is used in the right panel to predict the performance of the species in the field, at a specified PEC. Precondition for this method is that the test species and the test conditions are relevant to the expected field situation. This procedure is particularly useful for non-lethal endpoints (growth, reproduction, etc). A better toxicity test leads to less variation in the effects data, which reduces the uncertainty. Care must be taken to use this procedure on survival data. For these data, the variation between individuals of the tested population is not contained in the spread of the individual points, but is incorporated in the slope of the curve. If a test were conducted with clones of a species that are extremely alike, this would lead to a very steep survival curve (all individuals die at the same concentration). On the other hand, for non-lethal endpoints, the slope will be unaffected by using clones as this is a continuous endpoint.

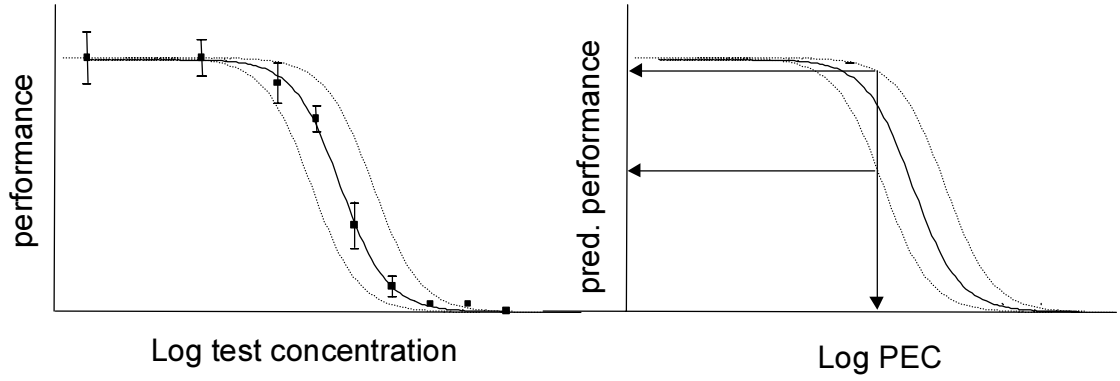


Figure A 12 Using dose-response relationships to predict performance of a species under field conditions.