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EUPHIDS, a decision support system for the admission of pesticides

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Preface

This report describes EUPHIDS, which stands for EUropean Pesticide Hazard Information and Decision support System. EUPHIDS is the result of a research project carried out with the support of the Environment Research Programme (1990-1994) of the European Union, under contract no. EV5V - CT92 - 0217. The system is meant to become an aid in the process of registering a plant protection product (pesticide) in the European Union, its member states and regions within the member states. The structure of the system and the implementation of the main modules are complete, and at this moment several submodules are being developed. The system is, therefore, not fully operational. Data provided by the system describe study areas (EU, D, I, Nl, Kreis Soest, Parco Sud di Milano, Hupselse Beek) and toxicological and ecotoxicological characteristics of eight pesticides. In order to establish a fully operating system on all scales and for all pesticides, more pesticide data and geographical information have to be gathered.

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Summary

The achievement of harmonization among European countries and their national groups of experts in the admission of pesticides is one of the most prominent aims of the European Union (EU) Directive 91/414. To this end, general criteria defining the relevant targets and the general procedures of assessment have been set down in the Uniform Principles. It should be noted, however, that the Uniform Principles do not provide detailed methods and procedures for the quantitative risk assessment of each relevant target. In particular, there is no specification of the methods by which the assessment can be linked to the specific characteristics of each area.

EUPHIDS (EUropean Pesticide Hazard Information and Decision support System) has filled this gap by adopting scientifically sound models of prediction for such phenomena as leaching, run-off, spray-drift and exposure of the operators and general population through diet. For each of these phenomena, algorithms have been developed that allow calculation and quantification of the dose delivered to the targets. Moreover, the models have been applied in such a way that the specific features of each environment and area can be taken into account at various spatial scales (continental, national, local); the spatial variation of the assessment can also be described with appropriate maps. EUPHIDS functions as a powerful tool to support decision-makers on pesticide registration at different administrative levels.

The system as presented in this report represents a first step in the realisation of prediction of effects of pesticides. It has not yet reached the complete level of maturity necessary for a standard decision method (tool). EUPHIDS is an open, flexible system which can easily be expanded with additional knowledge (data, models, rules) to provide the decision-maker with the information needed in line with the Uniform Principles. This system has been developed with the aim of integrating data collection, data analysis, data presentation and evaluation procedures. The structure of EUPHIDS and its main modules have been implemented in the current version described in this report. However, several new or alternative submodules are in development. The maturity of EUPHIDS as a fully operational system on all scales and for all pesticides will be determined by data availability and data and model quality.

EUPHIDS was built upon risk assessment schemes, including the models already developed and used in other contexts, as present in the Netherlands, Germany and Italy. The report describes all modules involved with special attention given to spatial modelling: the environmental part is based on grids, while the human assessment is based on dietary regions. The risks to humans and the environment, expressed as ratio of exposure to (no) effect levels, are presented in the form of maps. In this way, regions of high risk and also the component determining the risk can be easily identified.

A number of evaluation tools, beyond the Uniform Principle requirements, have been added, namely, ecosystem evaluation by means of safety factors or sensitivity distribution methodology. An aggregated evaluation is also offered using value functions to weight out different risks. Risks to human and the environment have not been aggregated.

Care should be taken in interpreting the results of the EUPHIDS calculations; the use of models provides an estimation of the consequences of pesticide use, but remains a prediction in which all uncertainties should be considered. Nevertheless, EUPHIDS offers clear insight to important information for making a decision about registration of pesticides - the risks - and is a very valuable tool in comparing risks between countries, regions and among different pesticides.

Samenvatting

In haar streven naar harmonisatie op het gebied van toelating van bestrijdingsmiddelen, zowel tussen de lidstaten als tussen nationale groepen van experts, heeft de Europese Unie Directive 91/414/EEC opgesteld. Annex 6 van deze Directive, de zogenaamde Uniforme Beginselen, geeft algemene criteria voor de toxicologische en ecotoxicologische risicobeoordeling, waaronder de te beoordelen doelen en algemene richtlijnen voor de te volgen procedures. De Uniforme Beginselen geven geen gedetailleerd voorschrift voor de kwantitatieve evaluatie van de risico's en ook geen richtlijnen over hoe risico's kunnen worden geëvalueerd afhankelijk van specifieke, regionale omstandigheden.
EUPHIDS (European Pesticide Hazard Information and Decision support System) is een beslissingsondersteunend systeem dat wel een gedetailleerde invulling geeft aan de kwantitatieve evaluatie van de risico's. In het systeem zijn modellen opgenomen voor de berekening van processen zoals uitspoeling en afspoeling, druppeldrift, blootstelling van werknemers in de landbouw en blootstelling van de mens via voedsel en drinkwater. De modellen zijn zodanig in EUPHIDS geïmplementeerd dat rekening wordt gehouden met verschillen in milieuomstandigheden op verschillende schaalniveaus (continentaal, nationaal, lokaal). De resultaten van de berekeningen worden weergegeven in kaarten voor de verschillende schaalniveaus en daarmee vormt EUPHIDS een krachtig ondersteunend systeem voor evaluerende instanties van de verschillende bestuurlijke eenheden.

EUPHIDS v1.0 is een volledig werkend systeem, dat echter niet uitputtend is in mogelijke berekeningsmethoden. Bovendien bevat het systeem slechts de geografische informatie van een aantal voorbeeldgebieden en zijn slechts voor een achttal stoffen chemische, biologische en (eco)toxicologische gegevens opgenomen. Op dit moment is EUPHIDS dan ook nog geen volwaardig systeem. Het systeem is echter zeer open (flexibel) opgezet, zodat aanvullende gegevens, maar ook alternatieve berekeningswijzen en beslissingsregels, eenvoudig kunnen worden toegevoegd. De gebruiker van het systeem kan middels een interface eenvoudig aangeven voor welk gebied hij berekeningen wil uitvoeren en welke berekeningswijzen en beslissingsregels hij wenst te hanteren.

EUPHIDS bouwt voort op beoordelingsmethodieken en modellen die in andere kaders in Europa, Nederland, Duitsland, Italie, enz. zijn ontwikkeld. Dit rapport beschrijft alle gebruikte methodieken en de manier waarop deze berekeningen ruimtelijk worden uitgevoerd. Blootstelling van milieucompartimenten wordt berekend per gridcel terwijl de blootstelling van de mens wordt berekend per dieet-gebied. Risico's worden weergegeven als de verhouding tussen de blootstellingsconcentratie en de concentratie waarbij (geen) effecten worden verwacht, zogenaamde risico-quotiënten. De resultaten worden weergegeven als kaarten, zodat eenvoudig die gebieden kunnen worden geïdentificeerd waarin een verhoogd risico aanwezig is.
Aan EUPHIDS is een aantal risico-evaluatietechnieken toegevoegd, die niet vermeld zijn in de Uniforme Beginselen, bedoeld om te komen tot een evaluatie van het risico voor afzonderlijke ecosystemen en het milieu als geheel. Deze technieken maken gebruik van verdelingen in gevoeligheid van organismen of van waarderingsfuncties, welke het

mogelijk maken afzonderlijke componenten te wegen. De afweging 'mens' ten opzichte van 'ecosysteem' is hierbij buiten beschouwing gelaten.

De resultaten van de berekeningen met EUPHIDS moeten met enige voorzichtigheid worden geïnterpreteerd; de berekende blootstellingen zijn schattingen met behulp van gegeven scenario's waarin onzekerheden zitten. Echter voor de vergelijking van verschillende middelen en van verschillende regio's en landen is het systeem zeer bruikbaar. Daarenboven wordt een volledig inzicht gegeven in de informatie die voor het nemen van een beslissing noodzakelijk is.

Zusammenfassung

Die Verwirklichung der Harmonisierung der Zulassung von Pflanzenschutzmitteln in den Ländern der Europäischen Union und deren nationalen Expertengremien ist eines der wichtigsten Ziele der EU-Richtlinie 91/414. Zu diesem Zweck geben die Uniform Principles ("Einheitliche Grundsätze") allgemeine Kriterien vor, die die hierzu relevanten Zielvorgaben und die allgemeinen Vorgehensweisen für die Zulassung definieren. Es muß jedoch betont werden, daß die Uniform Principles weder detaillierte Methoden und Verfahren zu einer quantitativen Risikoabschätzung für alle Schutzgüter vorgeben, noch eine Präzisierung der Methoden zur Verknüpfung dieser Risikoabschätzung mit spezifischen Eigenschaften einzelner geographischer Gebiete berücksichtigen.

EUPHIDS (EUropean Pesticide Hazard Information and Decision support System) schließt diese Lücke durch die Übernahme wissenschaftlicher Modelle für die Vorhersage von Prozessen wie Leaching, Run-off, Spraydrift sowie Exposition von Anwendern bei der Applikation und der allgemeinen Bevölkerung durch die Nahrungsaufnahme. Für jeden dieser Vorgänge sind Algorithmen entwickelt worden, die eine Berechnung und Quantifizierung von Wirkstoffkonzentrationen bzw. -dosen erlauben, denen die Schutzgüter (Mensch, aquatische und terrestrische Organismen, Grundwasser) ausgesetzt sind. Darüber hinaus sind die Modelle in einer Weise angewendet worden, daß die jeweiligen spezifischen Umwelteigenschaften der einzelnen geographischen Bezugsräume auf verschiedenen Maßstabsebenen (kontinental, national, lokal) berücksichtigt und die räumlichen Variationen der Abschätzung von Wirkstoffkonzentration bzw. -dosis in geeigneten Karten dargestellt werden können. EUPHIDS ist ein hervorragend geeignetes Instrument, Entscheidungsträger in der Zulassung von Pflanzenschutzmitteln auf verschiedenen administrativen Ebenen zu unterstützen.

Die Grundstruktur des EUPHIDS-Systemes sowie die Einarbeitung der wichtigsten Modelle sind zwar abgeschlossen, da aber derzeit noch einige Teilmodule weiterentwickelt werden, ist das System noch nicht vollständig fertiggestellt. Das hier vorgestellte EUPHIDS-System ist ein erster wichtiger Schritt hin zu einem komplett ausgereiften Instrument für den standardmäßigen Gebrauch zur Entscheidungsfindung in der Pflanzenschutzmittelzulassung. EUPHIDS ist ein offenes, flexibles System, daß sehr einfach mit neuen bzw. durch neue Erkenntnisse geänderte Informationen (Daten, Modellen, Regelwerken) aktualisiert werden kann, um Entscheidungsträgern in Anlehnung an die Uniform Principles ein jederzeit nutzbares Werkzeug zur Verfügung stellen zu können. Die Einsatzreife von EUPHIDS als voll funktionsfähiges System auf allen Ebenen räumlicher Auflösung und für alle Pflanzenschutzmittel ist jedoch sehr stark von der Qualität der Verfügbarkeit der Daten und Modelle abhängig. Verbesserungen auch der (räumlichen) Modellierung werden daher vorgeschlagen.

Dieses System ist entwickelt worden, um zusätzliche Zusammenstellungen, Analysen und Darstellungen von Daten sowie die dazu benötigten Bewertungsmethoden integrieren zu können.

Zukünftig könnte EUPHIDS durch das Hinzufügen neuer, alternativer Modelle zur Simulation der expositionsrelevanten Prozesse erweitert werden, und dann die Wahl der bevorzugten Methoden dem jeweiligen Nutzer des Systemes selbst überlassen.

EUPHIDS wurde auf der Grundlage von Bewertungsmethoden und Modellen entwickelt, die in den beteiligten Ländern Niederlande, Deutschland und Italien bereits eingesetzt worden sind. Dieser Bericht beschreibt alle im System eingebundenen Modelle und Module. Besondere Aufmerksamkeit wurde der raumbezogenen Anwendung der Modelle geschenkt: umweltbezogene Aspekte basieren auf der Grundlage von Rasterkarten, während die Beurteilung der humantoxikologischen Aspekte auf Ernährungsregionen aufgebaut ist. Die Risiken für Mensch und Umwelt, ausgedrückt als Quotient aus Umweltkonzentration und (No-)Effekt-Konzentration, werden in Form von Karten dargestellt. Auf diese Weise können einerseits Regionen identifiziert werden, für die ein hohes Risiko besteht, und andererseits jene Schutzgüter und Expositionspfade ermittelt werden, die zu diesem erhöhten Risiko führen.

Eine Reihe von bereits in EUPHIDS implementierten Bewertungsmethoden wie z. B. die Abschätzung des Risikos für Ökosysteme mit Hilfe von Sicherheitsfaktoren oder mittels Empfindlichkeitsverteilungsmethoden gehen über die Anforderungen der Uniform Principles hinaus. Zusätzlich ist auch eine zusammenfassende Bewertung des Umweltrisikos mit dem "Value-Function"-Ansatz möglich, über den die Möglichkeit besteht, die einzelnen Umweltkompartimente unterschiedlich zu wichten, um verschiedene Risiken differenziert in die Beurteilung einfließen lassen zu können. Risiken für Mensch und Umwelt können jedoch nicht zusammengefaßt bewertet werden.

Bei der Interpretation der mit EUPHIDS erzielten Resultate muß allerdings berücksichtigt werden, daß der Einsatz von Modellen nur Abschätzungen der realen Verhältnisse liefert, deren Unsicherheiten und Fehler nicht vernachlässigt werden dürfen.

Zumindest aber bietet EUPHIDS die Möglichkeit einer anschaulichen Darlegung des Entscheidungsfindungsprozesses, der zugrundeliegenden Datenbasis und der Ableitung der Risiken. Darüber hinaus ist es ein sehr variables Werkzeug für den Vergleich der Risiken auf verschiedenen räumlichen Maßstabsebenen und zwischen verschiedenen Pflanzenschutzmitteln.

Riassunto

Uno degli scopi principali della Direttiva Europea 414 è l'armonizzazione, tra le nazioni Europee e i gruppi nazionali di esperti, dei criteri per l'ammissione di prodotti fitosanitari. A tale proposito, i Principi Uniformi hanno stabilito criteri generali che definiscono i principali recettori e le procedure generali di valutazione. Va sottolineato, comunque, che i Principi Uniformi non definiscono metodi e procedure dettagliate per la valutazione quantitativa del rischio per ogni recettore e che non identificano alcuno strumento per legare la valutazione del rischio alle caratteristiche specifiche di un'area. EUPHIDS (European Pesticide Hazard Information and Decision support System) affronta tale problema utilizzando modelli scientificamente noti per la predizione di fenomeni quali il percolamento, il ruscellamento, la deriva, l'esposizione dei lavoratori e l'esposizione della popolazione generale attraverso la dieta. Per ognuno di questi fenomeni sono stati sviluppati algoritmi di calcolo che permettono la valutazione e la quantificazione della dose rilasciata ai ricettori. Inoltre i modelli sono stati applicati in modo da considerare la configurazione specifica di ogni comparto ambientale e quindi rappresentare, con mappe appropriate a diverse scale (continentale, nazionale, locale), la variazione spaziale della valutazione del rischio. EUPHIDS può essere quindi considerato un valido strumento di supporto alle decisioni nella registrazione dei prodotti fitosanitari a diversi livelli amministrativi.

Il sistema presentato in questo rapporto è una prima realizzazione e non ha ancora raggiunto il completo livello di maturità necessario allo sviluppo di uno strumento decisionale. EUPHIDS è un sistema flessibile e aperto e può essere facilmente ampliato per fornire al decisore le informazioni necessarie, secondi i Principi Uniformi. Questo sistema è stato sviluppato per integrare la raccolta, l'analisi e la presentazione dei dati e le valutazione delle procedure. Nel futuro EUPHIDS potrà essere ulteriormente migliorato con l'aggiunta di altri modelli e quindi con la possibilità di scelta, da parte del decisore, di metodologie diverse per la valutazione di un singolo processo.

EUPHIDS è stato sviluppato secondo schemi di valutazione del rischio già inclusi in modelli disponibili e in uso in altri paesi quali l'Olanda, la Germania, l'Italia ecc. Questo rapporto descrive tutti i moduli considerati. Viene posta una particolare attenzione alla modellistica "spaziale": il modulo ambiente è infatti basato su "grid" mentre la valutazione del rischio per la salute umana fa riferimento a regioni alimentari. I rischi per l'uomo e per l'ambiente, espressi come rapporto tra l'esposizione e i (no) effect level, sono rappresentati tramite mappe. In questo modo possono essere facilmente identificate sia le regioni ad elevato rischio sia le componenti determinanti il rischio.

Al sistema sono stati inoltre aggiunti un certo numero di strumenti di valutazione, quali la valutazione dell'ecosistema per mezzo dei safety factor o della metodologia di distribuzione di sensibilità, che vanno oltre gli scopi dei Principi Uniformi. Si ha inoltre la possibilità di aggregare le valutazioni per pesare i diversi rischi utilizzando le "value functions". Non è stata considerata la possibilità di aggregare il rischio per l'uomo con quello per l'ambiente. E' tuttavia necessaria una certa cautela nell'interpretazione dei risultati dei calcoli di EUPHIDS; l'uso dei modelli, infatti, fornisce una stima ma rimane pur sempre una predizione caratterizzata da molte incertezze.

EUPHIDS offre comunque una chiara rappresentazione delle informazioni necessarie alle decisioni - valutazione dei rischi - ed è uno strumento prezioso per il confronto dei rischi nelle diverse nazioni, regioni e per diversi prodotti fitosanitari.

La struttura di EUPHIDS è completa, ma, allo stato attuale, diversi sottomoduli devono ancora essere sviluppati rendendo così il sistema parzialmente incompleto. Il raggiungimento di un elevato livello di funzionalità di EUPHIDS a tutte le diverse scale e per tutti i prodotti fitosanitari dipenderà dalla disponibilità dei dati e dalla qualità dei modelli. E' consigliabile un miglioramento nella modellistica "spaziale".

1. Introduction

1.1. Background information

The European Union (EU) and its Member States are in the process of developing policies to prevent food, air, soil, groundwater and surface water from (further) contamination with pesticides and to diminish, as much as possible, adverse impacts on the environment and public health. All countries of the EU have some kind of evaluation procedure for the registration of plant protection products (subsequently referred to as pesticides), however, the evaluation procedures differ considerably, both with respect to aspects evaluated, and the degree of explicity of the procedure. In its Directive 91/414/EEC, the EU initialised the harmonization of pesticide registration legislation. Part of this harmonization process is the development of the so-called 'Uniform Principles' (Annex VI of Directive 91/414/EEC), which aims at uniform procedure for the registration of pesticides in the EU (including the information required from industry to properly evaluate a pesticide, recommended guidelines for the conduct of experiments and unique (uniform) criteria for decision making). The Standing Committee for Plant Protection is responsible for the evaluation of pesticides on the European scale.

Directive 91/414/EEC (Commission of the EU, 1991) concerns the placing of plant protection products on the market. The purpose of this Directive is to regulate and harmonize the requirements for authorising plant protection products on the European Union level. The Directive states, for example, that a plant protection product is not authorised unless:

- it is sufficiently effective;
- it has no unacceptable effects on plants or plant products;
- it does not cause unnecessary suffering and pain to indicated vertebrates;
- it has no harmful effect on human or animal health, directly or indirectly (e.g. through drinking water, food);
- it has no unacceptable influence on the environment, particularly regarding:
  i. its fate and distribution in the environment, particularly contamination of water including drinking water and groundwater;
  ii. its impact on non-target species.

Annexes II and III of Directive 91/414/EEC state the requirements for the dossier to be submitted for the authorisation of active substances and of plant protection products, respectively. Annex VI states the Uniform Principles for the evaluation of plant protection products.

The Uniform Principles (UP) have been established in Directive 94/43/EEC (Commission of the EU, 1994). The Directive states which environmental and health aspects have to be evaluated, how they have to be evaluated and the criteria that have to be met.

Some general principles for evaluations are that they:

- should be performed by best scientific and technical means;
- should consider the intended use of the pesticide (i.e. dose, frequency, method and time of application) in normal agricultural practice (according to the rules of Good Agricultural Practice);
- should consider agricultural, plant health and environmental (including climatic) conditions in areas in which the product will be used;
- should consider possible uncertainties in the data and, accordingly, evaluate average and realistic worst case conditions;
- upon use of models, these models should:
  - i. include all relevant processes;
  - ii. use realistic parameters and boundary conditions;
  - iii. be calibrated against data from relevant test circumstances;
  - iv. be relevant for the area where the pesticide is to be used and
- should evaluate all relevant metabolites, transformation and reaction products.

1.2. Objectives

EUPHIDS (EUropean Pesticide Hazard Information and Decision Support System) has been developed as an open decision support tool, and quantitatively evaluates environmental and human health effects caused by the use of pesticides on different spatial scales. This implies that:

- all manner of ecotoxicological and human health evaluations can be conducted;
- additional models or meta-models can be easily incorporated;
- other data can be easily imported;
- various spatial scales can be evaluated for a pesticide, expanding or limiting its potential use.

EUPHIDS is a flexible tool for designing thematic maps which identify and rank vulnerable regions with respect to groundwater contamination, environmental risks to terrestrial and aquatic organisms as well as health risks to agricultural workers and the general population (Table 1.1).

Table 1.1. Toxicological and ecotoxicological targets considered in EUPHIDS.

Toxicological targets	
-	general population (consumers)
-	agricultural workers (applicators, farmers)
Environmental targets	
-	individual organisms in soil and surface water
-	terrestrial ecosystems
-	aquatic ecosystems
-	groundwater
-	environment

EUPHIDS follows the Directives 91/414/EEC and 94/43/EEC and goes beyond its requirements. It evaluates the distribution of a pesticide over different environmental compartments after its release according to good agricultural practice. Environmental and human exposure are compared with toxicity data for humans, aquatic and terrestrial organisms. Possible short term (acute) and long term (chronic) effects are considered. The use of EUPHIDS for a given area can support the relative evaluation of pesticides, although automatic procedures for ranking of pesticides are not yet available.

In EUPHIDS, special attention is paid to spatially variable processes, fulfilling the requirement as stated in the Directives. Environmental exposure is modelled spatially on a grid basis for the compartments soil (treated field), (shallow) groundwater and surface water (major parts still to be implemented). Human exposure is modelled per dietary region. The results of the modelling are given in maps showing concentrations and evaluations on either a grid base for the environmental module or on the basis of human dietary regions. The results may, subsequently, be aggregated to match the desired administrative area. EUPHIDS offers, moreover, several tools which are beyond the minimum requirements as laid down in the Directives. These include:

- The risk assessment for aquatic and terrestrial ecosystems as a whole. This uses, for example, safety and decision support factors according to the Environmental Protection Agency (EPA) or extrapolation techniques according to the sensitivity distribution method (Aldenberg and Slob, 1993).
- The risk assessment for aquatic and terrestrial ecosystems, and the system as a whole, according to value-function techniques (Beinat, 1995).
- Spatial analyses, such as filtering and smoothing techniques, to gain insight into the variability of the risks dependent on the area considered.

It has been decided to treat ecosystems separately from risks to humans, including agricultural workers because of:

- the nature of available information and differences in spatial resolution (larger resolution for the ecotoxicological targets);
- the type of risk evaluation (single targets for human health vs. single, but also multiple, targets for ecosystems);
- the type of risk acceptance (acceptable risk to ecosystems is higher than to humans);
- the lack of knowledge of mutual trade-offs and
- ethical reasons.

Pesticide registration is not only a matter for the European Commission (Standing Committee), but for national, regional and local tiers of government as well. Therefore, different spatial scales are incorporated into the system: the European, national (Germany, Italy and the Netherlands) and (example of the) regional scale. Because of differences in data availability on the different scales the results of the calculations and evaluations are, at the moment, not necessarily the same, however, as much consistency as possible is aimed at.

It should be noted that the main purpose of the evaluation is to assess the risk posed by active ingredients in the pesticide products. However, since the active ingredients are marketed in specific formulations, the composition of which is highly relevant to the risk assessment process, EUPHIDS also considers the formulations in relation to some factors in the assessment (especially agricultural workers). The formulations also have some influence on the behaviour of the product in the environment, but this is almost exclusively on secondary processes which are not modelled in EUPHIDS (e.g. volatilization, uptake through leaves, distribution in water bodies).

1.3. Some basic definitions

Hazard is defined as the inherent potential of a substance to cause adverse effects. Risk is defined as the probability of a substance to cause adverse effects under given circumstances of use. The risk quotient[1] between the Predicted Environmental Concentration (PEC) and the (No) Effect Level ((N)EL) is used as an approximation for the risk posed by a pesticide to humans, organisms or ecosystems. The main definitions used in EUPHIDS are given in Table 1.2; Appendix A1 gives all the definitions and abbreviations.

Table 1.2. Some basic definitions used in EUPHIDS (after USES, 1994)

Hazard assessment
the identification of the adverse effects which a substance has an inherent capacity to bring about

Dose-response assessment
the estimation of the relationship between dose or concentration and the incidence and severity of an effect

Exposure assessment
the determination of the emissions, pathways and rates of movement of a substance and its transformation products to estimate the concentrations or doses to which human populations, or ecological systems and populations, are or may be exposed

Risk evaluation
the process designed to estimate the incidence and severity of the adverse effects likely to occur in a human population or environmental compartment due to actual or predicted exposure

Risk quotient
the quotient of the actual or predicted exposure and the (predicted) no effect exposure level. In EUPHIDS this risk quotient is used as an approximation for risk

1.4. The structure of the report

Chapter 2 introduces the functional requirements of the EUPHIDS system. The methodology of environmental assessment is dealt with in Chapter 3 where the environmental evaluation will also be addressed. The methodology for human exposure assessment and evaluation (general population and agricultural worker) is outlined in Chapter 4. Chapter 5 addresses the spatial data and GIS aspects of the project. In Chapter 6 a guided tour through EUPHIDS is given to illustrate the functionality and use of EUPHIDS as a decision support tool in pesticide registration. Chapter 7 lists items of discussion with respect to EUPHIDS and its methodological elaboration. Finally, in Chapter 8, conclusions are drawn and recommendations given, along with some perspectives on future developments.

[1] Defined as PEC/(N)EL. In the literature the term TER (toxicity exposure ratio = (N)EL/PEC), the reciprocal value of the risk quotient, can also be found.

2. Overview of EUPHIDS

2.1. *Introduction*

The use of pesticides forms an integral part of modern agriculture. It is supposed to assure farmers high yields and good quality of crops. The use of certain pesticides however poses a threat to environmental and public health. In the decision making process of the farmer these external effects are in general not taken into account. Governments and public authorities, on the contrary, may use several instruments to prevent negative effects on man and the environment. Examples are the admission procedures and the economic incentives or disincentives to the use of a substance. The direct regulation through admission procedures is still the most applied option. Through the current admission procedures government has the possibility to ban harmful pesticides. The admission of a pesticide is a very complex, multi-disciplinary process. The most important disciplines are agronomy, economy, toxicology, ecotoxicology and sociology (see Figure 2.1). Registration in general will be granted if beneficial effects outweigh possible negative effects. Negative effects mostly are associated with risks or threats posed on man and the environment. This research project covers only a part of all decisions to be taken; it deals with toxicological and ecotoxicological aspects, taking into account established policies in agriculture, environment and human health. This is outlined in Figure 2.1.

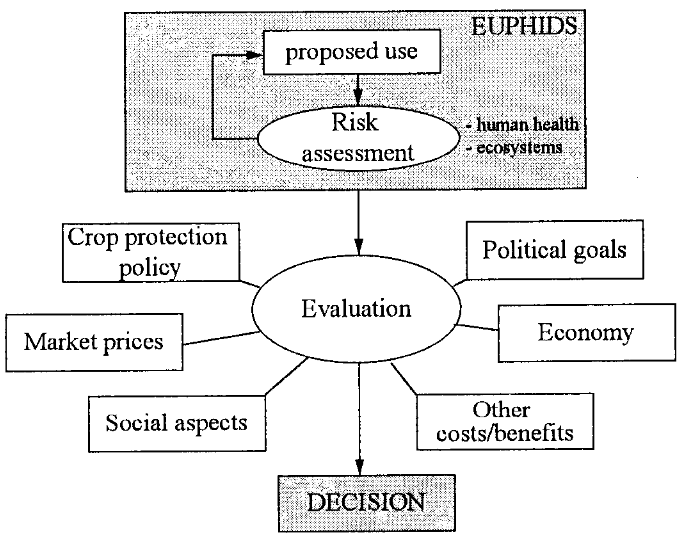

Figure 2.1. General outline of the decision making procedures on the admission of pesticides (EUPHIDS covers the parts in the shaded area box).

The decision support system, EUPHIDS, is developed to assist policy makers and registration officers in their decisions on pesticide admission. The objective is to provide more integrated, more transparent and regionalized information. This chapter describes the functional and methodological design of the system. It also provides a structure for the upcoming chapters in this report.

2.2. *Towards a decision support for the admission of pesticides*

At this moment there are large differences between admission procedures in the various member states of the EU. In general, there is a lack of transparency and decision rules are unclear. Different models are applied to calculate the environmental and human health exposure and often different reference values are used to assess the risks of the pesticide under study. In addition, it is not clear how the integration of the various risk categories takes place resulting in the final decision. Are effects on terrestrial ecosystems, for instance, as important as those on groundwater? This leads to situations where, for instance, a certain pesticide is banned in one country and admitted in the other. Admission procedures are in general also characterised by the fact that regional differences only to a limited extent are taken into account. Effects in one area can thus be overestimated and in another area underestimated.

The use of uniform decision procedures and rules makes the decision making process transparent. Through the incorporation of the spatial distribution of effects (e.g. by spatial varying model parameters) policy makers obtain more realistic information on risks of pesticides in their particular region and thus are able to define and implement policy measures to control and limit these risks.

The Uniform Principles partly accommodate the shortcomings mentioned here. They aim at standardising admission procedures in Europe by comprising a general outline and guidance on the evaluation of effects. The major objectives of protection dealt with in the Uniform Principles are: groundwater, aquatic and terrestrial ecosystems outside the target area and on the field as well as human health. A regional aspect is coming into consideration by Article 10 of the Directive. According to the guidelines a first evaluation of pesticides will take place at the European level. A ban at this level will overrule decisions taken at lower political levels (see Figure 2.2).

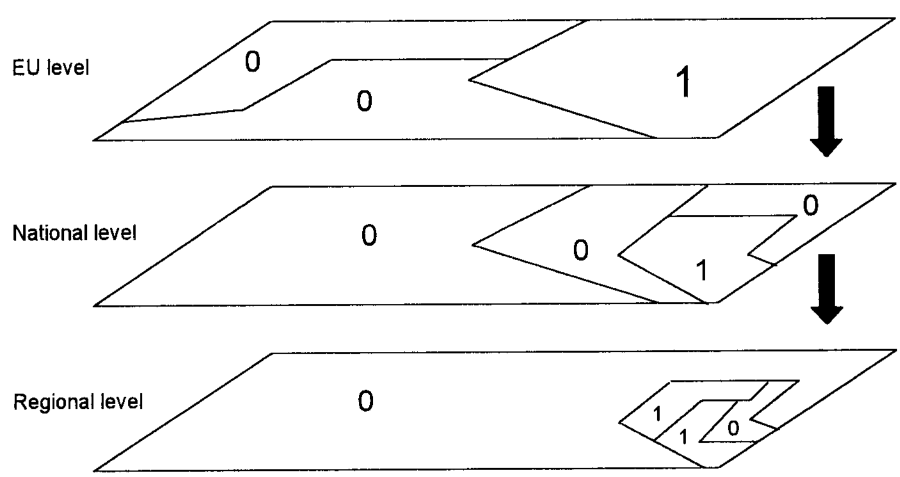

Figure 2.2. Schematic overview spatial decision model (1 = authorisation, 0 = no authorisation).

On the other hand the Article states that a country can deny an EU authorisation, if national or regional environmental conditions are different from the EU average.

2.3. EUPHIDS: a pesticide admission support tool

The decision support system, EUPHIDS, is developed to assist policy makers and registration officers in their decisions on pesticide admission. It follows the guidelines set by the Uniform Principles with respect to pesticide risk assessment and evaluation. It consist of a number of features intending to provide better, more transparent, information to overcome part of the shortcomings noticed above. In particular:

- EUPHIDS offers decision makers in an easy accessible computer environment a structured decision model for the identification of pesticide risks based on the Uniform Principles. Such information can be used in pesticide admission procedures.
- Besides the guidelines set in the Uniform Principles, EUPHIDS offers additional functionality to apply other (more strict) evaluation procedures as well as to integrate (environmental) effects.
- At different spatial scales (Europe, national, regional), EUPHIDS calculates and presents regional effects, which enables the identification and localisation of sensitive areas.
- EUPHIDS integrates knowledge and information from various disciplines involved in pesticide risk assessment and evaluation. In this project a number of representative methods and techniques have been developed and implemented in the system. Spatial data layers from several (test) regions have been collected and linked to the system to test and demonstrate its functionality. The design of EUPHIDS is characterised by a relative 'open' structure, which enables the implementation of other risk assessment and evaluation methods and techniques, other (new) pesticides or other regions.

Figure 2.3 shows in a schematic way the structure of the decision support tool at a single decision level. The pesticide with its properties, application dose and spatial parameters are the input for the exposure assessment. This results in information on the Predicted Environmental Concentration (PEC) surface water (for fish, daphnia and algae; short term and long term), the PEC topsoil (for earthworms; short term and long term), the PEC groundwater, the Estimated Daily Intake (EDI) of the general population and the dermal and inhalation exposures of the agricultural worker. Except for the exposure of the agricultural worker this information is regionalized and presented in maps. Subsequently, this information can be evaluated in order to assess the risk. Exposure levels are confronted with various short and long term single species (No)-Effect Levels ((N)EL). Besides the Uniform Principles also other procedures can be used. Additionally, integration of environmental risk is supported to assess the risk on the ecosystem level and the combined ecosystems level. The output of EUPHIDS is a series of maps, indicating the spatial distribution of the degree of pesticide risk for the various receptor groups.

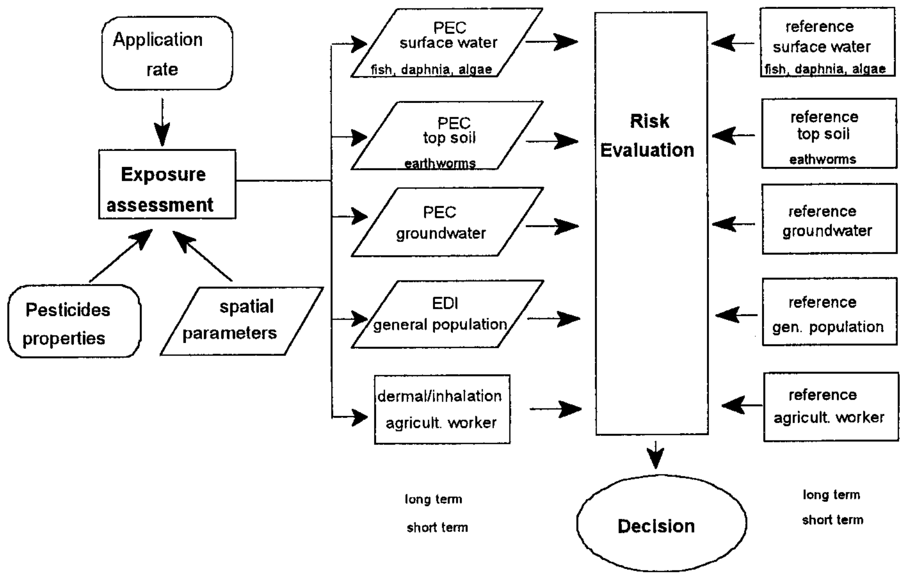

Figure 2.3. Structure of EUPHIDS.

2.4. Risk assessment and evaluation.

2.4.1. Risk assessment

In good agricultural practice pesticides are used according to a prescribed dose. This prescribed dose usually varies for instance with crop, soil type and climate, but essentially is known within a factor of two. Using less pesticide in general leads to an insufficient treatment of the pest; using more pesticide has an over-effect and is economically inefficient. The dose is the starting point for exposure calculations of man and environment. Targets of the exposure assessment are indicated in Figure 2.3. To calculate these endpoints EUPHIDS encompasses a number of exposure routes: interception, spraydrift, run-off, leaching and human health exposure routes. Figure 2.4 gives an overview of the exposure routes and receptor groups considered.

All calculations are scenario-type calculations performed for:

- the amount in the plough layer immediately after application and a certain period after application;
- the amount leaching to groundwater (below the level of 1 m - soil surface);
- the amount reaching surface water via drift and/or run-off;
- the amount taken up by the general population via food and drinking water;
- the amount taken up by workers in agriculture via direct exposure.

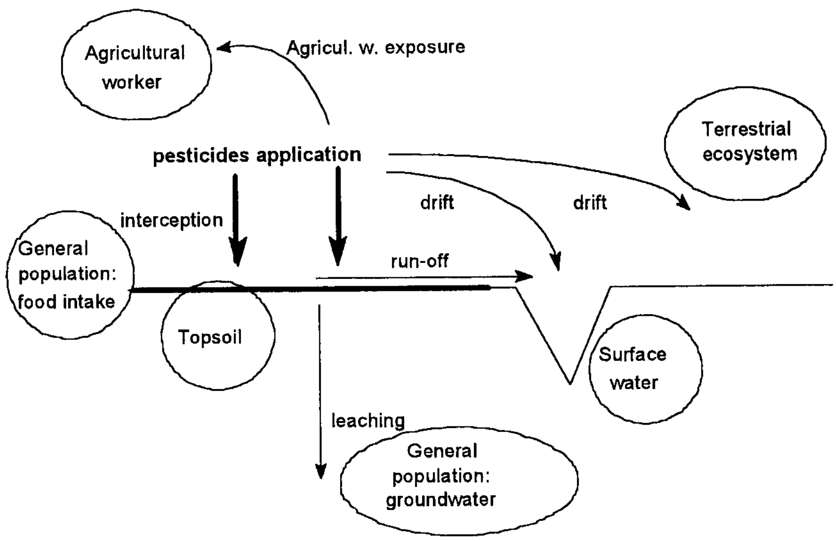

Figure 2.4. The main pesticide dispersion routes and related receptor groups taken into account in EUPHIDS.

In the system special attention is paid to those estimations that have spatial variability. Estimations on intrinsic pesticide properties (for instance whether bound residue formation limits will be exceeded) is not incorporated in the system. These aspects have to be considered in pesticide registration, but as they have no spatial variability a simple yes/no registration decision can be made on the basis of one or a few experiments.

2.4.2. Risk evaluation

The data for risk evaluation is obtained from the registration dossiers or from literature. On the basis of these data evaluation takes place. In the 7th amendment of guideline 67/548/EEC the basis for the risk definition in ecotoxicology is given. Risk is evaluated from the quotient PEC/(N)EL (Predicted Environmental Concentration over No Effect Level). The quotient is called the risk quotient; the risk is equal to 1 if the ratio PEC/(N)EL = 1. This basis is used throughout EUPHIDS[2]; an estimated concentration or load is compared to the maximum concentration or load that does not lead to adverse effects. This principle is not only used for ecotoxicological aspects, but also for toxicological aspects: an estimated (daily) intake is compared to levels that are supposed to cause no harm to humans.

(N)ELs are also calculated for aquatic and terrestrial ecosystems, or for the environment as a whole. These extrapolations go beyond the requirements given by the Uniform Principles, but may be helpful in taking ultimate decisions and comparing compounds to each other. The EPA method (taking into account safety factors) and sensitivity distribution techniques are implemented to assess ecosystem level risks. Value functions are introduced in EUPHIDS as a technique for integrating the effects on multiple environmental compartments.

[2] As mentioned before, the term Toxicological Exposure Ratio (TER) is also used in the practice of pesticide evaluation. TER is defined as (N)EL/PEC.

2.5. *Spatial data in EUPHIDS*

The spatial decision model of Figure 2.1 depicts various decision levels: the European level, national and regional levels. At all these levels different decision makers are involved in the reduction of pesticide risk, for instance by using hierarchical admission procedures.

The resolution of the information required for the admission of the pesticide differs at different spatial levels. At European scale, the global identification and localisation of pesticide risks is probably sufficient to support the admission procedure. At the regional and local scale, on the other hand, much more detail is needed. In general terms, the degree of detail needed depends on two aspects: the spatial scale of the decision domain and the spatial variability of the processes of dispersion and exposure to the pesticide.

Most environmental processes incorporated in EUPHIDS are regionalized. This holds for the dispersion and fate of the substance in the environment and for the exposure of the general population. The models and algorithms used in EUPHIDS are applied at the grid-cell level[3]. As an example, the leaching of a pesticide in groundwater can be represented as a map. This map shows, for each grid-cell, the amount of the substance which can be found in groundwater after a certain time and under a set of modelling conditions. The result is obtained calculating the leaching of the pesticide within each grid-cell independently.

Geographic Information Systems (GIS) play an important role in EUPHIDS as concerns collection, storage, management, analysis, integration and presentation of data. One of the most appealing functions of GIS is to store and integrate data from different sources into a spatial environment. The design of the spatial data model is a pre-requisite for the regionalization of the exposure and risk levels. At the current development stage, EUPHIDS includes several layers of spatial data for Europe, the Netherlands, Germany, Italy. In order to test the system also at the local scale, EUPHIDS includes three small test areas: the Hupselse Beek (Netherlands), Kreis Soest (Germany) and Parco Sud di Milano (Italy).

2.6. *Developing EUPHIDS: some notes on the strategy used*

Two main phases can be distinguished along the development of EUPHIDS (cf. Figure 2.5):

1. the development of models for pesticide dispersion, exposure and risk evaluation;
2. the integration of models and spatial data in EUPHIDS.

The first phase is preparatory. It involves the development of the spatial data model stored in a GIS together with all the other models included in the system. The integration

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[3] A grid-cell is a (uniform) square portion of the area under evaluation (for instance a 2.5 km square area) and is the spatial basis of all calculations in EUPHIDS. All input and output maps in the environmental part of EUPHIDS are represented in a raster format through grid-cells. The size of the grid-cell can be different at different spatial levels (regional, national, European; see Chapter 5). Grid-cells are replaced by uniform diet regions in the calculation and evaluation of human health exposure due to food intake.

of the two results in the regionalization of effects. More in particular, the following models have been developed:

- Models for calculating the exposure level for different environmental compartments on the basis of drift, interception, leaching and run-off of the pesticide;
- Models to compute human exposure with distinction between general population exposure (due to food residues and drinking water) and agricultural worker exposure (due to direct contact and inhalation);
- Evaluation models, to evaluate human and environmental exposures against acceptable levels. These models use the results of the previous ones as an input.
- Presentation model, to support the visualisation and the statistical analysis of maps and other outputs. Map analysis techniques, like filtering, are also implemented to increase insight in spatial patterns of risk.

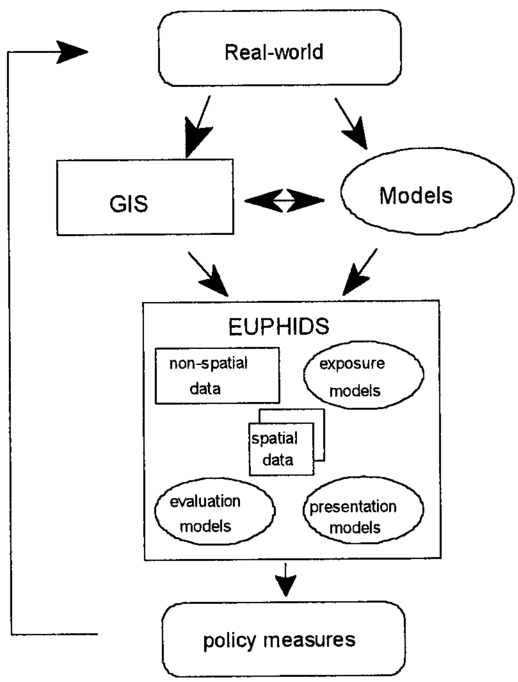

Figure 2.5. The development and organisation of EUPHIDS.

A large share of these models have been developed on a 'heavy' hardware and software platforms (workstations), especially designed for development purposes. For instance, the development and testing of the leaching models and the computations of leaching parameters have been based on a UNIX workstation. The same holds for most of the spatial database.

During the second phase the models developed and the data collected are processed and transferred into to a flexible, transparent and user-friendly environment which becomes EUPHIDS. In contrast to the platforms used for development, this environment, is a 'light' information environment with specifically tailored functionality. In this environment the components developed (exposure models, evaluation models, presentation models and (spatial) data) are integrated. However, only the sections of the models necessary for pesticide evaluation are used. Therefore, in some cases EUPHIDS offers the access to complete models and all related parameters. In other cases, only components or even model outcomes previously computed are used (for instance, the outcomes of the leaching model). This increases the computation performance of the system, making possible the integration of several models in one "light" system. EUPHIDS is also designed in such a way that the incorporation of other models or of other additional regions can be easily implemented.

3. Methods for environmental risk assessment and evaluation

3.1. Introduction

According to Council-Directive 94/43/EC (1994) Member States have to consider all aspects of the environment, including biota, in the evaluation of the fate, distribution and probable effects of plant protection products, including the extent of short-term and long-term risk to be expected for aquatic and terrestrial non-target organisms after use of such products according to the proposed conditions of use. Environmental compartments like aquatic and terrestrial ecosystems, groundwater and air as well as the agricultural area itself may be exposed to pesticides by different pathways (Figure 3.1). In terms of pesticide exposure assessment, for environmental compartments in the immediate vicinity of a treated area and for this area itself, the quantitatively most important exposure routes are:

1. Direct application of a pesticide on the field in form of spray, granules or treated seeds.
2. Spraydrift to adjacent ecosystems in the course of spray application.
3. Run-off from a treated area during torrential rain events.
4. Leaching of a plant protection products to groundwater by water percolating through soil.

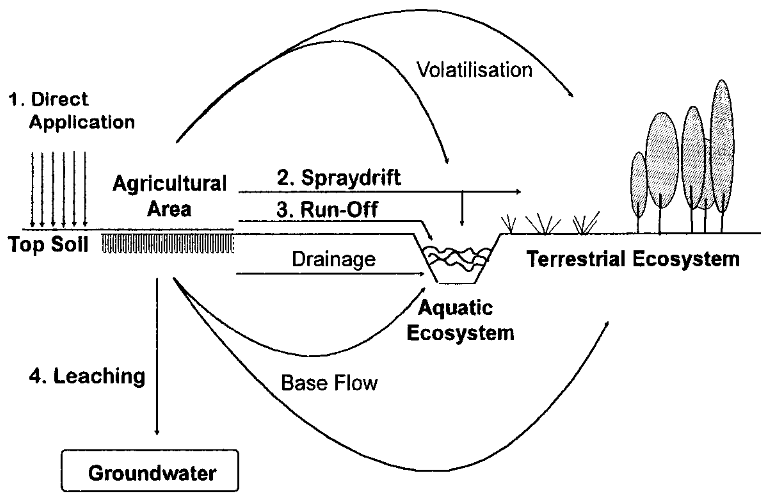

Figure 3.1. Exposure Pathways for Aquatic and Terrestrial Ecosystems and Groundwater.

Other pathways like volatilisation with subsequent deposition and base flow are quantitatively less important for the exposure of non target areas in the close neighbourhood of application spots whereas volatilisation is the most important exposure route for remote regions far away from the locations of pesticide use like, e.g., the arctic (Herrchen et al., 1994). Drainage might be of relevance for the exposure of surface water but up to now no satisfactory models to assess drain exist. Thus, direct application, spraydrift, run-off and leaching are the considered exposure routes in EUPHIDS.

The general architecture of the EUPHIDS exposure and ecotoxicological risk assessment module is visualised in Figure 3.2. For each grid cell predicted environmental concentrations (PECs) for different environmental compartments like top-soil, groundwater, and surface water are calculated under consideration of the relevant exposure routes. Input data for these PEC calculations is:

- data related to the pesticide properties and use,
- scenario type data (for large regions) describing characteristics of representative soils, climates or ecosystems, and
- spatial data provided by the GIS-environment as digitised maps. This data is for example some soil parameters, topography, climate, and land use.

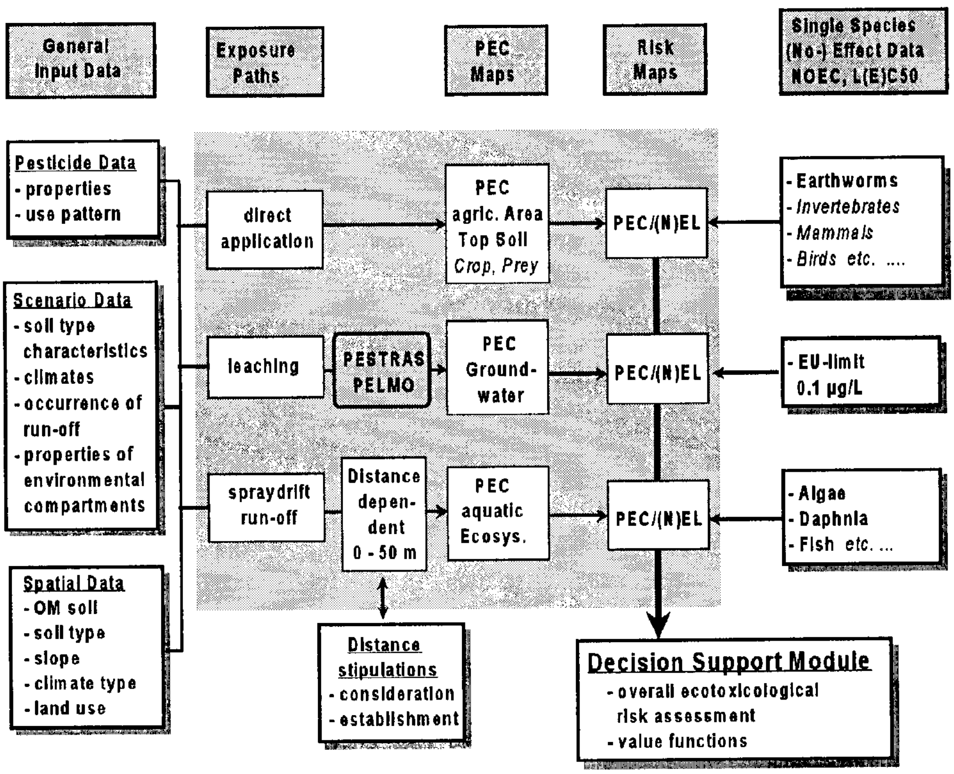

Figure 3.2. EUPHIDS Environmental Exposure and Effects Assessment Module (Abbreviations: OM soil: organic matter of soil; PEC: predicted environmental concentration; (N)EL: (no)-effect level).

Pesticide leaching to groundwater is calculated by leaching models. The PEC for surface water of aquatic ecosystems is estimated considering spraydrift and run-off[4]. An exposure and risk assessment for terrestrial non-target ecosystems adjacent to the treated field is not explicitly included in the assessment module. Instead of assessing risk to terrestrial ecosystems outside the field a risk assessment for terrestrial organisms living

[4] Since the amount of pesticide that may reach the aquatic ecosystem is, among other factors, dependent on the distance between the ecosystem and the trated area, this distance can be optionally set between 1 and 50 m by the user. Thus, distance stipulations already imposed can be considered in the course of EC calculation, or such measures can be established interactively by running the system with different field-surface water distance settings.

on the treated field itself will be implemented in the course of the system improvement[5]. The reason for this is the lack of data for representative organisms of specific terrestrial ecosystems. Birds, mammals, and earthworms, for which data has to be provided and therefore can currently be used as indicator organisms for probable pesticide impacts on terrestrial ecosystems, must already be protected from adverse effects under conditions that occur on treated fields. Because potential pesticide concentrations can reasonably be expected to be higher on a treated field than in an adjacent terrestrial ecosystem, it seems not very meaningful to perform two risk assessments since a potential risk for the mentioned species on terrestrial non-target areas can be denied if adverse effects are unlikely under conditions occurring on the treated field.

The PECs for the different environmental compartments are compared with the respective (no-)effect level data ((N)EL), as stated in the "Uniform Principles": e.g. EC_{50}, LD_{50}, NOEC, PNEC, HC_5^{95}) for short term and long term toxicity which are based on single species tests. The resulting PEC/(N)EL ratios serve as indicators for the environmental risks due to the use of the assessed pesticide. The risk quotients can be visualised as risk maps and additionally serve as input in the decision support module where the overall assessment of the pesticide is performed by aggregating and weighing several partial aspects and results of the pesticide assessment.

3.2. Calculation of Predicted Environmental Concentrations

The environmental assessment module of EUPHIDS is based on broadly accepted methods which are also the basis for the assessment according to the "Uniform Principles" (Council-Directive 94/43/EC). These are, e.g., scenario-approaches and exposure models to estimate predicted environmental concentrations (PEC).

The amount and quality of pesticide related physico-chemical data necessary to run the system do not differ from those obligatory in current admission procedures in several European countries. However, this data is supplemented with spatial variables provided by the GIS-module of EUPHIDS. The spatial variables are related, e.g., to soil, climate, topography, and land use.

Information from maps and scenario assumptions in connection with pesticide data (physico-chemical properties and use data) is used to calculate spatially differing PECs. PECs are calculated for different time intervals to account for acute and chronic exposure. Pesticide removal processes like degradation, adsorption and advection are considered by using first order decay functions. The PECs for top-soil, groundwater and aquatic ecosystems in each single grid cell can be transformed to and displayed as PEC maps.

3.2.1. Calculation of PECs for Aquatic Ecosystems

Due to lacking knowledge on location, frequency of occurrence, type, size and hydrological and chemical parameters of surface waters in the real environment a realistic worst case scenario approach is used to calculate PEC in surface waters. For that

[5] See the Appendix A7 "Estimation of PECs and pesticide risks for organisms of the terrestrial environment"

purpose it is assumed that (i) in each gridcell aquatic ecosystems are present in 1 to 50 m distance from the treated area and that (ii) pesticide emissions from that area reach a standard ditch of 25 cm depth (Figure 3.3). Partitioning of pesticides between water body and sediment is not considered since no spatial information on organic carbon content of sediments is available. For short term exposure the omission of sediments in the PEC calculation is a worst case approach because a probable diminution of the water phase concentration due to adsorption of a pesticide onto organic matter in sediment is not accounted for. However, long term PECs may be underestimated by that procedure since probable pesticide releases from sediment are neglected.

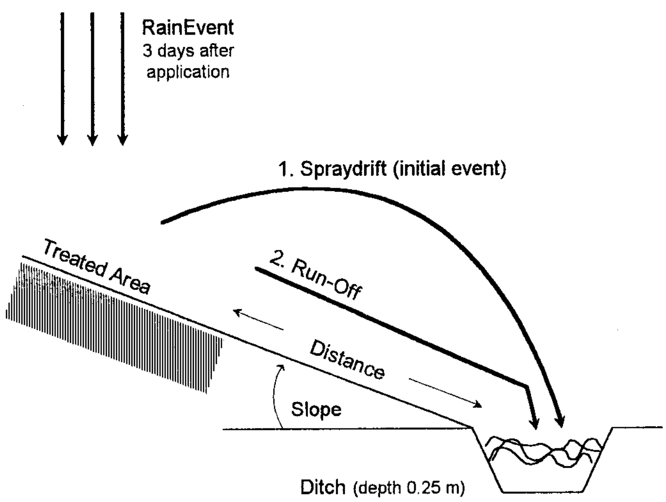

Figure 3.3. Spraydrift and run-off emissions to a ditch.

The distance between treated agricultural area and the standard-ditch can be chosen by the user of the system. The most important exposure pathways for aquatic ecosystems adjacent to a pesticide treated area are spraydrift and run-off. Thus, exposure originating from these pathways needs to be calculated and finally to be integrated to obtain a PEC for surface water. If a pesticide is not applied as spray (application e.g. as granules or as treated seeds or directly into soil) spraydrift is not considered in the course of PEC calculation. Thus, in such cases, run-off is the only exposure path accounted for (the user of EUPHIDS can choose to include/exclude the spraydrift and run-off modules in the calculations).

Spraydrift emission is considered the initial event occurring immediately upon application of the pesticide. A run-off event is assumed to take place with a certain time delay (3 days) after spraying[6]. Additionally, the EUPHIDS user-interface offers the opportunity to select scenarios in which the calculation of surface water PECs is based either on spraydrift or on run-off emissions alone. It is intended to account for multiple pesticide applications in the future system development[7].

[6] See section 3.2.3 (Run-off) below for details and explanations.
[7] See The Appendix A6: "Multiple applications, in the calculation of PEC in ditches".

3.2.2. Spraydrift

The amount of spraydrift reaching non-target areas is dependent on:

- Distance from the area of application
- Mode of application (formulation, technical equipment)
- Crop (height, growth stage)
- Weather (e.g. wind speed)

As shown in Figure 3.4 which is based on experiments performed in Germany (Ganzelmeyer et al., 1995), spraydrift emissions to non-target ecosystems decline with the distance to the application area. Further, they exhibit considerable variability for different crops and application techniques.

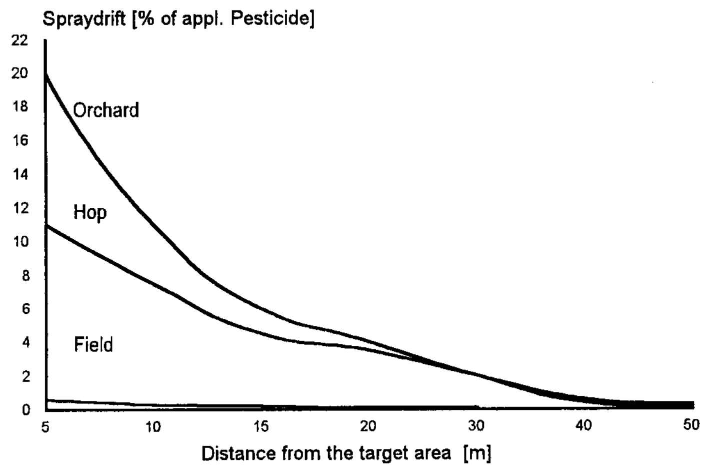

Figure 3.4 Pesticide spraydrift dependent on crop-type and distance from the target area. The spraydrift is expressed as a percentage of the aerial mass (dose) reaching the treated field.

The pesticide spraydrift deposition is calculated as follows:

$$\text{deposition } (= DOSE_{drift}) = DOSE_{nominal} * f_{drift} \qquad (3.1)$$

In which:

f_{drift} = spraydrift fraction, which is dependent on crop, growth stage and distance from the target area

In EUPHIDS the spraydrift fraction is read from tables implemented in the database module. Three options are available: two tables are based on German experimental results (Table 3.1, Table 3.2). These tables comprise the 50^{th} and 95^{th} percentiles of a series of experiments performed in collaboration by German authorities and the industry (Ganzelmeyer et al., 1995).

The third table (Table 3.3) is based on Dutch data which are also used in the Dutch "Uniform System for the Evaluation of Substances" (USES, 1994). The German tables allow to choose the drift factor dependent on the distance between ecosystem and application area as well as dependent on crop and growth stage. The Dutch data is predominantly based on expert judgement and only suitable for situations where the target is immediately adjacent to the sprayed area. This data is based on experiments in which the ditches started at a distance of about 1 meter. However, Dutch data accounts for some more application types than the German data.

Table 3.1. German drift table I; 95th percentiles of spraydrift deposition.

distance from the treated area [m]	vineyard deposition [% of applied dose] early	late	orchards deposition [% of applied dose] early	late	hop deposition [% of applied dose]	vegetable etc. deposition [% of applied dose] H < 50 cm	H > 50 cm	field deposition [% of applied dose]
5	1.6	5.0	20	10	12.5	0.6	5	0.6
10	0.4	1.5	11	4.5	9.0	0.4	1.5	0.4
15	0.2	0.8	6	6	5.0	0.2	0.8	0.2
20	0.1	0.4	4	1.5	4.0	0.1	0.4	0.1
30	0.1	0.4	2	0.6	2	0.1	0.2	0.1
40	0.1	0.2	0.4	0.4	-	-	0.2	-
50	0.1	0.2	0.2	0.2	0.3	-	0.2	-

Table 3.2. German drift table II; 50th percentiles of spraydrift deposition.

distance from the treated area [m]	vineyard deposition [% of applied dose] early	late	orchards deposition [% of applied dose] early	late	hop deposition [% of applied dose]	vegetable etc. deposition [% of applied dose] H < 50 cm	H > 50 cm	field deposition [% of applied dose]
5	1.7	2.7	12.1	5.4	7.9	0.5	2.7	0.5
10	0.4	0.9	5.8	2.2	3.5	0.2	0.9	0.2
15	0.2	0.4	2.9	1.2	2.7	0.0	0.4	0.0
20	0.1	0.2	1.9	0.75	1.2	0.0	0.2	0.0
30	0.0	0.1	0.9	0.3	0.5	0.0	0.1	0.0
40	0.0	0.0	0.1	0.1	0.2	-	0.0	-
50	0.0	0.0	0.1	0.1	0.1	-	0.0	-

Table 3.3. Dutch spraydrift table (only suitable for situations where the target is adjacent to the sprayed area).

Application Mode	Drift Fraction	Application Mode	Drift Fraction
spot application	0.005	arboriculture	0.100
row application	0.005	aeroplane	1.000
bare soil	0.010	glasshouse	0
crop < 0.25 m	0.010	ditch	0.100
crop > 0.25 m	0.020	......continued	.....

3.2.3. Run-Off

The second important exposure route for surface water is run-off from pesticide treated fields after heavy rain events (Figure 3.5). The occurrence and the extent of run-off is dependent on the topography of the landscape (slope), the soil texture and the intensity of the rain event. The amount of pesticide that may be translocated into surface waters is further dependent on the distance between the treated area and the receiving ecosystem as well as on the elapsed time between pesticide application and onset of rainfall. Under condition of Good Agricultural Practice it is not likely that run-off will occur earlier than 3 days after application because farmers will listen to the weather forecast and will avoid the application of pesticides if heavy rainfall is announced because the impact of the pesticide is limited then. Therefore, it is assumed in the scenario for run-off calculation that run-off will not occur earlier than three days after pesticide application. The amount of pesticide still present in the top layer of the soil three days after application is liable to run-off. Further, the probability for occurrence of run-off events in flat regions and areas with very permeable soil (on the basis of the classification into sandy or stony soils) is assumed to be zero.

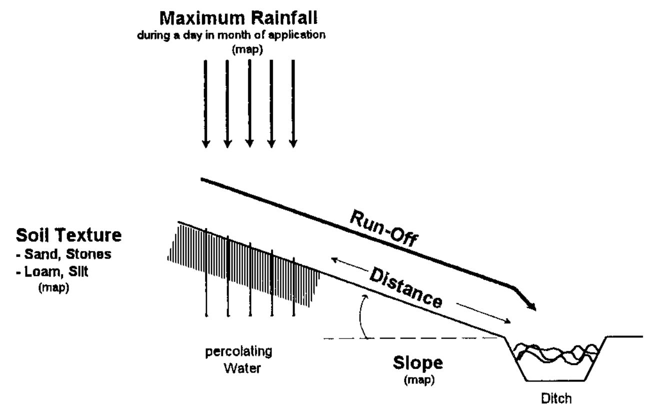

Figure 3.5. Exposure of aquatic ecosystems by run-off

The spatial information necessary to calculate run-off emissions is supplied as map information by the GIS environment of EUPHIDS (Sand and Stone map, Soil Organic Matter map, Slope map, Maximum-Rainfall map). Soil type, slope and rainfall are the three maps which determine the spatial variability of run-off events.

The percentage of pesticide loss by run-off is calculated by an empirical equation derived from experimental results (Klöppel et al., 1994). Important variables are the sand and stone factor, the slope factor, the rainfall factor and the sorption constant of the pesticide to soil organic carbon.

$$P_r = F_{ST} * F_s * F_r * \{0.55 * \log (K_{OC}) + 1.47\} \qquad (3.2)$$

In which:

P_r = Fraction of pesticide lost by run-off (%).

K_{OC} = Sorption constant (kg * dm^{-3}): $K_{OC} = 1.72 * K_{OM}$.

F_{ST} = Soil type factor. This factor indicates whether a soil is susceptible to run-off. The factor is an attribute of the soil map (0 for sand and stones, 1 for clay, loam and silt).

F_s = Slope factor. This factor is a function of the slope and is calculated as follows: $0.124*SL+0.0082SL^2$ (SL = slope [%] taken from CORINE SLEC map).

F_r = Rainfall factor. Map input is, for each month in which pesticides may be applied, the arithmetic mean of the maximum precipitation within a day over the past 30 years (peak events). Thus, maximally 12 maps could be available. Currently maximum rainfall in may is the only map functional in EUPHIDS. Rainfall maps for other months still have to be included.

Not the amount of rainfall itself but the excess which cannot be soaked up by the soil is determining whether run-off takes place. It was empirically found that run-off starts after a rainfall of approximately 17 mm. Thus, the rainfall factor is calculated as:

$$F_r = 0.0208 * RE + 0.00011 * RE^2 \qquad (3.3)$$

with:
RE (rain excess) = average maximum daily rainfall (R_{max} mm) - 17 mm.

On the basis of its sorption constant (K_{OC}) and on the organic matter content of soil, a pesticide may be predominantly translocated dissolved in the water phase or adsorbed on eroded particles. The organic matter content of soil is a spatial variable. Therefore, the fractions of particle-bound and water-dissolved pesticide need to be estimated for each gridcell in order to calculate the concentration of the pesticide in the respective fractions. The soil organic matter content is map input in the calculation.

a) Pesticide sorption onto soil particles in suspension:

$$Q = F_c * K_{OC} * \frac{M_{OM}}{100} * c_s \qquad (3.4)$$

In which:
Q = Sorption capacity
F_c = Sorption-Desorption factor depending on slope length (set 2)
K_{OC} = Sorption coefficient of pesticide to organic carbon ($dm^3.kg^{-1}$)
M_{OM} = Organic matter content of soil (%) (map input)
c_s = Concentration of soil particles in water ($g.L^{-1}$)

b) Pesticide fractions in:

(i) sediment and ii) water

$$F_{sed} = \frac{Q}{Q+1} \qquad (3.5) \qquad\qquad F_{aq} = \frac{1}{Q+1} \qquad (3.6)$$

The pesticide concentration in run-off water and eroded sediment is dependent on the pesticide dose in the soil, the percentage of washed-off pesticide, the fraction of pesticide dissolved in the run-off water phase, and the run-off depth, which is the amount of run-off water that is assumed to leave the application area.

$$c_{aq} = P_r * DOSE_{soil} * \frac{F_{aq}}{D_r} \quad (3.7) \qquad c_{sed} = P_r * DOSE_{soil} * \frac{F_{sed}}{D_r} \quad (3.8)$$

In which:

D_r = Run-off depth (l/m^2; expressed in mm). Due to empirical evidence the run-off depth is set to be 10 mm less than 47% of the initial amount of precipitation. $D_r = (0.47 * R_{max}) - 10$.

Only c_{aq} is used to calculate the PEC in surface water since it is assumed that c_{sed} is not bioavailable and therefore not effective.

3.2.4. Calculation of PEC Surface Water

Figure 3.4. visualises the assumed rise and fall of the pesticide concentration in ditch water with time: From an unknown background level, which is currently assumed to be zero because no or hardly any information is available, a concentration peak in water is reached due to spraydrift immission. Caused by several removal processes such as, e.g., sorption to organic matter, evaporation, biodegradation and dilution, the pesticide concentration drops down with time. As a second impact, the run-off event causes a new concentration peak. Depending on environmental conditions and pesticide properties, this peak may be higher or lower than the initial peak caused by spraydrift alone. However, this second concentration peak is considered as $PEC_{short\ term}$ when both spraydrift and run-off are taken into account as relevant exposure routes. If in the EUPHIDS user interface only spraydrift is selected as exposure route the first concentration peak caused by spraydrift alone is considered as $PEC_{short\ term}$. In order to avoid underestimation of $PEC_{short\ term}$, it is therefore advisable to run the exposure assessment module twice with both spraydrift and spraydrift plus run off as exposure routes.

Opposite to the short term concentration in surface water, $PEC_{long\ term}$ is calculated as mean concentration over a certain exposure interval. This approach was chosen since for a chronic exposure assessment the average concentration is relatively more relevant than short lasting initial concentration peaks. The duration of the long term exposure interval depends on the duration of the ecotoxicological tests the PEC is related to (usually between 72 h for algae to 21 d for fish). PECs are calculated for each grid cell and displayed as surface water PEC maps.

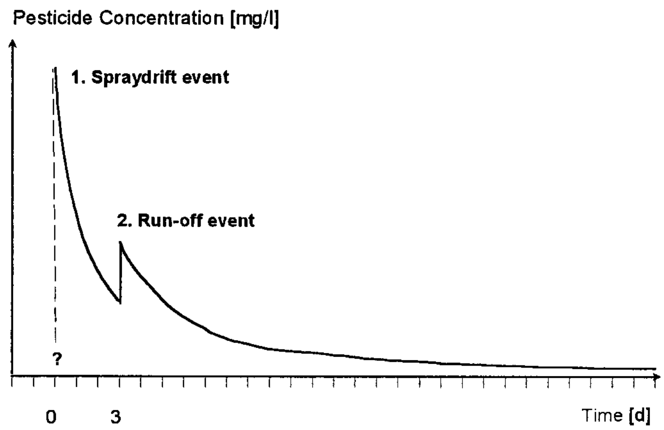

Table 3.4. Pesticide concentration in a ditch as a result of spraydrift and run-off emissions.

3.2.4.1. Calculation of $PEC_{short\ term}$

$PEC_{short\ term}$ in surface water is calculated either as initial concentration due to spraydrift and run-off or due to spraydrift alone:

i) due to spraydrift

$$c_{0,d} = \frac{100 * DOSE_{nom} * f_{drift,\ dist}}{d} \qquad (3.9)$$

ii) due to spraydrift and run-off

$$c_{0,r} = c_{t,d} + \frac{P_r * DOSE_{soil} * F_{aq}}{D_r} \qquad (3.10)$$

In which:

$c_{0,d}$	= Initial concentration due to spraydrift (mg/l)
$c_{0,r}$	= Initial concentration due to spraydrift and run-off (mg/l)
$c_{t,d}$	= Concentration due to spraydrift at the time of the run-off event (3 days after spraying): $c_{t,d} = c_{0,d} * e^{(-K_T * t)}$ (See equations 3.11 to 3.13)
100	= Conversion factor kg/ha $\Rightarrow$ mg/m^2
$DOSE_{nom}$	= Nominal pesticide dose (kg/ha)
$DOSE_{soil}$	= Pesticide dose that reaches the top soil (kg/ha) (See equation 3.19)
$f_{drift,\ dist}$	= Distance and crop type dependent fraction of spraydrift
d	= Depth of the ditch (m)
P_r	= Fraction of pesticide lost by run-off (See equation 3.2)
F_{aq}	= Fraction of pesticide dissolved in run-off water. See equation 3.1.1.5
D_r	= Run-off depth (mm) (See equations 3.5 and 3.6)

3.2.4.2. Calculation of $PEC_{long\ term}$

The long term PEC for surface waters is calculated taking into account removal processes which lead to a decrease in pesticide concentration over time. The decay of pesticides is considered to obey first order kinetics. Then, the decay-rate constant is:

$$K = \ln 2 / DT_{50} \qquad (3.11)$$

In which:
K = First order rate constant (d^{-1})
DT_{50} = Half life time (d)

The variables which can influence the pesticide decay are (i) Evaporation (K_v), (ii) Degradation (K_{bio}), and (iii) Advection (K_a) which result in the overall decay constant:

$$K = K_v + K_{bio} + K_a$$

Since evaporation and biodegradation of pesticides are temperature dependent processes, the decay rate constant K is adjusted by a temperature correction factor f_t according to an approximation to the Arrhenius equation (Boesten & van der Linden, 1991):

$$K_T = (f_t * \ln 2) / DT_{50} \quad (3.12)$$

In which:
K_T = Temperature corrected degradation rate constant
f_t = Temperature correction factor; $f_t = e^{(\gamma * (t - t_{ref}))}$
t = Average temperature of the month of application
t_{ref} = Temp. at which degradation in water was investigated (default: 20° C)
γ = Constant (default: 0.08)

The pesticide concentration at any given time is expressed by the equation:

$$c(t) = c_0 * e^{(-K_T * t)} \quad (3.13)$$

In which:
c(t) = Pesticide concentration in water at time t (mg/l)
c_0 = Initial pesticide concentration in water at time t_0
K_T = Overall first order decay constant (d^{-1})
t = Time elapsed since occurrence of spraydrift or run-off event (d)

Average concentration over time is obtained by integration:

$$\bar{c} = \frac{c_0 * \{1 - e^{(-K_T * t_{exposure})}\}}{K_T * t_{exposure}} \quad (3.14)$$

In which:

$\bar{c}$ = Time averaged pesticide concentration in water over $t_{exposure}$ days (mg/l)
$t_{exposure}$ = Exposure-time interval (duration of ecotoxicological test or default) (d)

The time intervals of exposure for which the long term PECs are calculated depend on the duration of the single species tests they are related to. So, for algae this $t_{exposure}$ may be 72h, for daphnia 14d, and for fish 28d. The exposure intervals used by EUPHIDS are either those automatically retrieved from the pesticide toxicity tests database (defaults) or user input.

3.2.4.3. Combination of a spraydrift and a run-off event

The following points in time are relevant:

1 t_0 (d) The time of application (spraydrift emission)
2 t_{r0} (d) The time at which the run-off event takes place
3 $t_{exposure}$ (d) The duration of the exposure (= duration of single species test)

The calculations start with estimating the average concentration c_d (mg/l) over the time period $t_{r0} - t_0$:

$$\bar{c}_d = \frac{c_{0,d} * \{1 - e^{(-K_T * (t_{r0} - t_0))}\}}{K_T * (t_{r0} - t_0)} \qquad (3.15)$$

In which:

c_d = Time averaged concentration in water due to spraydrift before occurrence of run-off event over $t_{r0} - t_0$ (=3) days (mg/l)
$c_{0,d}$ = Initial concentration due to spraydrift (mg/l)

Equation 3.15 is fully equivalent to equation 3.14. Therefore, the residue concentration at the time of the start of the run-off event ($c_{r,d}$ mg/l) is calculated using an adapted form of equation 3.13:

$$c_{r,d} = c_{0,d} * e^{(-K_m * (t_{r0} - t_0))} \qquad (3.16)$$

The average concentration over the period of the run-off event, $\bar{c}_r$ (mg/l), is obtained by substituting $c_{r,d}$ and $c_{0,r}$ into equation 3.13:

$$\bar{c}_r = \frac{(c_{0,r} + c_{r,d}) * \{1 - e^{(-K_T * t_{exposure})}\}}{K_T * t_{exposure}} \qquad (3.17)$$

The average concentration resulting from spraydrift and run-off over the exposure interval ($t_{exposure}$) is the arithmetic mean:

$$\bar{C} = \frac{(t_{r0} - t_0) * \bar{c}_d + (t_{exposure} - (t_{r0} - t_0)) * \bar{c}_r}{t_{exposure}} \qquad (3.18)$$

3.2.5. Calculation of PEC for Top Soil of the Treated Area

Plant protection products may reach the top soil either after spraying or by direct application into soil or upon applying granules or treated seeds. In case of direct application into soil and applying granules or treated seeds it is assumed that 100 % of the nominal pesticide dose (kg/ha) will reach the soil whereas in case of spraydrift the amount of pesticide finally reaching the soil is dependent on application losses like evaporation during spraying and interception by plants growing on the sprayed area.

In EUPHIDS, the default for loss during spray application is set to 10 % to account for all losses not accounted in other calculations, such as residues in tanks, volatilisation etc. (cf. also USES, 1994) This option can be changed in EUPHIDS. Interception by plants is dependent on species and developmental stage of the crop at the time of spraying. It is not yet adjustable in the EUPHIDS user-interface, but this functionality will be implemented with high priority in the future improvement of the system. To achieve this, a table with species and developmental stage dependent figures for spray interception by the crop will be stored in EUPHIDS and made available to the choice of the user (Table 3.5). The dose reaching the top soil is then calculated as follows:

$DOSE_{soil}$ (kg/ha) = (1-f_{int}) * (1-f_{al}) * $DOSE_{nom}$ (kg/ha) (⇒ spray application) (3.19)
$DOSE_{soil}$ (kg/ha) = $DOSE_{nom}$ (kg/ha)(⇒ application into soil, granules, treated seeds)

In which:

f_{int} = Fraction of pesticide intercepted by plants (Table 3.5; This fraction is not yet adjustable in EUPHIDS. Thus, the current results of PEC top soil calculations are those for pesticide applications on bare soil (f_{int} = 0). An option to consider interception by plants is to add an appropriate figure from the table to the application loss and change manually the default setting for this parameter in the Initialisation Menu of EUPHIDS. Notice that with this operation the application loss for groundwater and the surface water PEC calculations will also change, affecting the PECs for these compartments. The effect can be studies by running the system twice with different application loss settings for ground and surface water and for top soil.

f_{al} = Application loss, e.g. due to evaporation during spraying (default=0.1=10 %)

Like for surface water, short term and long term concentrations are calculated. The $PEC_{short\ term}$ is the initial concentration after pesticide application and $PEC_{long\ term}$ is the average concentration over a time interval. The length of this time interval is dependent on the exposure time of the toxicity test the PEC will be compared with. In the scenario for calculation of PEC_{soil} it is assumed that pesticides are evenly distributed in the upper 5 cm ($PEC_{short\ term}$) or 20 cm ($PEC_{long\ term}$) of soil, irrespective whether they are applied as spray, granules or treated seeds.

Table 3.5. Intercepted fractions of pesticide spraydrift.

Crop	Intercepted Fraction	Crop	Intercepted Fraction
default	0.11	corns_1st_month	0.11
potatoes_1st_month	0.22	corns_full_growth	0.89
potatoes_full_growth	0.89	grassland	0.44
fruit_spring	0.44	sprouts_full_growth	0.78
fruit_full_foliage	0.78	onions_full_growth	0.56
peas_1st_month	0.11	bulbs	0.50
peas_full_growth	0.78	tubers	0.50

3.2.5.1. PEC_{soil} short term

PEC_{soil} short term is calculated as follows:

$$PEC_{soil,st}\ (kg * kg^{-1}) = \frac{10^{-4} * DOSE_{soil}}{TL_{ts} * {}^{b}\rho_s} \qquad (3.20)$$

In which:

10^{-4}	= Factor to convert kg/ha to kg/m^2
$DOSE_{soil}$	= See equation 3.19
Tl_{ts}	= Thickness of top soil (0.05 m)
${}^{b}\rho_s$	= Bulk density of dry soil (kg/m^3); default 1.5 kg/m^3

3.2.5.2. PEC_{soil} long term

PEC_{soil} long term is the integrated time averaged concentration in the plough-layer calculated by means of a first order decay function.
The first order pesticide degradation rate (K) in top soil is:

$$K = \ln 2 / DT_{50} \qquad (3.21)$$

with DT_{50} as pesticide half-life time in soil. Since the biodegradation of pesticides in soil is very much dependent on soil temperature (microbial activity), a temperature correction factor according to an approximation to the Arrhenius equation is included (Boesten & van der Linden, 1991):

$$K_T = (f_t * \ln 2) / DT_{50} \qquad (3.22)$$

In which:

K_T = Temperature corrected degradation rate constant

f_t = Temperature correction factor; $f_t = e^{(\gamma * (t - t_{ref}))}$

- t = Average temperature of the month of application
- t_{ref} = Temp. at which the degradation in soil was investigated (default: 20° C)
- γ = Constant (default: 0.08)

The integrated time averaged concentration in the plough layer can now be obtained as:

$$PEC_{soil,lt}\ (kg/kg) = c_{0,pl} * \frac{(1 - e^{-K_T * t_{exposure}})}{K_T * t_{exposure}} \qquad (3.23)$$

with:

$c_{0,pl}$ = Initial concentration in the plough layer. $c_{0,pl}$ is calculated the same way as $PEC_{soil,st}$ except that the soil depth TL_{ts} is 0.2 m (see equation 3.20)

K_T = Temperature dependent first order degradation constant

$t_{exposure}$ = Exposure-time interval (default: 28 d, European convention; or duration of ecotoxicological test)

3.2.6. Leaching of Pesticides to Groundwater

In EUPHIDS, the leaching of a pesticide is calculated in a meta-modelling approach. This means that no leaching model itself is part of the EUPHIDS software but its results for an application dose of 1 kg/ha and a range of pesticide properties and environmental conditions related to soil and climate. These results are stored as leaching-tables and are subject to further modifications in the EUPHIDS program (e.g. adjustment of predicted pesticide concentration in groundwater to soil organic matter content of the actual grid cell and to the applied dose). This open environment of EUPHIDS offers the opportunity to use any suitable model for the calculation of leaching. Simply, leaching-tables with the respective results for the basic pesticide properties and environmental conditions need to be calculated externally with the model and added to the system.

Beside implementation of this open environment feature, the meta-modelling approach was chosen to keep the run-time of the leaching module as short as possible in order to assure the suitability of EUPHIDS as a decision-making tool. Pesticide leaching depends on many parameters related, e.g., to its physico-chemical parameters, soil properties, climate, and agricultural practice (Table 3.6). Thus, the chosen modelling approach is useful to avoid extended processing times when a PC-platform is used. The model output just needs to be adjusted by the program but not generated by computation of complex processes and huge amounts of data.

Since the modelling of leaching is very much dependent on spatial information related to soil properties, climate and agricultural practice (Table 3.6), a very large number of leaching tables would be necessary to reflect all combinations occurring at different spots in the real world. To limit the number of tables to a manageable amount and since not all data related to soil properties and climate, which is needed to calculate PEC groundwater, is available in the form of digitised maps (e.g. relevant soil parameters in different layers, thickness of soil and daily data for climate parameters; see Table 3.6), it was chosen to create so called soil-climate scenarios. For this purpose a number of representative soils (criteria: covered area, use as arable land) were characterised by the parameters needed as input for the leaching models. All soil types not covered by this procedure were assigned to the most closely related of the characterised soils. Similarly, areas considered to be uniform with respect to climate were created and combined with the selected soils by overlaying the resulting soil and climate maps. Representative crops (soil use) were chosen additionally for each of the soil and climate combinations to correct the soil water balance for plant evapo-transpiration when calculating pesticide leaching. Thus, the combination of a soil type, its site specific use (crop) and the spatial climate resulted in a number of spatially different soil-climate scenarios. These soil-climate scenarios were determined for each scale of spatial resolution (European, national, local) [8].

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[8] For scenarios and data see also Appendices A4 “Meta-information on spatial data“ and A3 “Spatial scenarios for pesticide leaching“

For Europe, e.g., these are 12 soil-climate areas resulting from the combination of 12 climates and 5 soils (Table 3.7). The European climate areas are defined in terms of a mean annual temperature range and a certain precipitation surplus (e.g. $8 < T < 10$ and $p_{netto} > 500$ mm/yr) (Figure 3.6). As representative soils the most important according to the above mentioned criteria were chosen. The definition and determination of the national and local scenarios was performed by the respective national groups participating in the project. Criteria were the reflection of principal spatial differences in soil properties, soil use and climate as well as the already mentioned reduction of spatial variability to a manageable extend. So, for Germany, 5 representative soils types were selected and combined with 9 climates to result in 13 soil-climate areas (Table 3.8, Figure 3.7). The 2 Italian soil-climate scenarios result from the combination of 2 climates and 2 soils (Table 3.9, Figure 3.8), and the Dutch scenarios base on one climate and 7 soils (Table 3.10, Figure 3.9). The local scenarios (Hupselse Beek, NL; Parco Sud, I; Kreis Soest, D) do not differ in climate but only in soil properties and use.

Table 3.6. Compilation of some parameters influencing pesticide leaching to groundwater

Physico-chemical properties of the pesticide	Soil properties	Climate	Agricultural practice
e.g.: - sorption constant (K_{OM}) - degradation rate (DT_{50})	e.g. in different layers: - organic matter cont. - pH - cation exchange capacity - clay, sand and loam content - bulk density	e.g.: - temperature - precipitation - rel. humidity	e.g.: - pesticide dose - frequency of applications - spring or fall application - crop and crop rotation mode

The leaching of plant protection products was calculated by two leaching models, the Dutch leaching model PESTRAS (Tiktak et al., 1994) and the German model PELMO (Klein, 1994, 1995). PESTRAS is based on PESTLA (Boesten & van der Linden, 1991), the officially adopted model for calculating leaching in the pesticide admission procedure in The Netherlands. PELMO is the official model used in Germany. Nonetheless, their output is somewhat different. PESTRAS calculates the maximum concentration in the upper meter of groundwater and PELMO the mean concentration at 1 m depth below the soil surface.

By means of both models leaching-tables for hypothetical pesticides differing in sorption constants to organic matter (K_{OM}) and half life time in soil (DT_{50}) were calculated for all soil-climate areas at each level of spatial resolution and added to the EUPHIDS database (Figure 3.10). Each of these tables covers a K_{OM} and DT_{50} range from 1 to 200 (dm^3/kg and days, respectively). The content of the leaching tables is the concentration in groundwater resulting from the application of 1 kg/ha, dependent on K_{OM} and DT_{50} of the pesticide and on the climatic and edaphic conditions described by the respective soil-climate scenario. The EUPHIDS user interface offers the opportunity to choose between the tables calculated by means of PESTRAS or PELMO.

In practice, the calculation of the PEC groundwater of a single grid cell is then performed by the EUPHIDS program as follows (Figure 3.11):

1. First, the soil-climate area is identified in which the grid-cell is located
2. Then, the leaching table with respect to the chosen leaching model, the time of application, and the soil climate area is selected
3. An apparent K_{OM}^* for the pesticide is calculated. That means, the K_{OM} of the pesticide is corrected by the ratio between the organic matter content of the soil in the gridcell and the organic matter of the soil reference scenario

$$K_{OM}^* = K_{OM} * \frac{\% \, OM_{gridcell}}{\% \, OM_{reference}} \quad (3.24)$$

4. The concentration of pesticide in groundwater is finally obtained by linear interpolation in the DT_{50} - K_{OM} table and corrected for the applied pesticide dose.

$$PEC_{groundwater} = \text{Interpolated figure from leaching table} * Dose_{soil} \quad (3.25)$$

Long term pesticide concentrations in groundwater calculated according to the above mentioned procedure can be displayed as PEC maps in the EUPHIDS system.

Table 3.7. Soil-Climate Scenarios for Europe.

Europe							
No	**Geography**	**Temperature Class (° C)**	**Precipitation Excess Class (mm)**	**Representative Soil**	**Organic Matter (% OM)**	**Representative Crop**
1	south-west Spain, south Portugal	15-20	< 250	loam	< 3	wheat
2	east Spain	10-15	< 250	coarse sand	< 3	barley
3	north Portugal, north Spain, southern France	10-15	> 250	coarse sand	< 3	maize, wheat
4	central France	10-15	< 250	loam / sand	< 3	wheat
5	north-east France, Benelux, Germany, Denmark, south Norway/Sweden, west Norway	5-10	< 250	loam / sand	< 4	barley
6	Great Britain	5-10	> 250	loam (elevated groundwater)	< 4	barley
7	south east Sweden	5-10	< 250	sand	< 4	wheat
8	Norway	0-5	> 250	coarse sand	< 4	wheat
9	Sweden	0-5	< 250	coarse sand	< 4	wheat
10	north Italy, north Greece	10-15	> 250	coarse sand	< 3	maize
11	south Italy, Sicily, Sardinia, south Greece, Crete	15-20	> 250	clay	< 2	wheat
12	Alps: Austria, Switzerland	data not available				

Table 3.8. Soil-Climate Scenarios for Germany.

Germany					
No	**Soil type**	**Geology**	**Geography**	**Climate station**	**Representative Crops**
1	Marshy Gleyosols	Marine sediments	Influence of tides at the North Sea cost	Husum	Spring: Winter wheat Fall: Winter wheat
2	Cambisols	Glacial sediments	Northern Baltic Sea Coast	Husum	Spring: Rye Fall: Rye
3	Podzols	Glacial sediments and sediments in the surrounding of glaciers (sandy sediments)	North East Podzol Region	Teterow	Spring: Winter barley Fall: Winter barley
4	Podzols	Glacial sediments and sediments in the surrounding of glaciers (sandy sediments)	South East Podzol Region	Berlin	Spring: Winter barley Fall: Winter barley
5	Podzols	Glacial sediments and sediments in the surrounding of glaciers (sandy sediments)	Western Podzol Region	Hamburg	Spring: Potatoes Fall: Winter barley
6	Cambisols (and Dystrict Cambisols)	Glacial sediments	Berlin Region	Berlin	Spring: Rye Fall: Rye
7	Luvisols	Loess	Northern and North Eastern Loess Region	Magdeburg	Spring: Sugar beet Fall: Winter wheat
8	Rendzinas (and Calcic Cambisols)	Mesozoic lime stones	Northern Karst Region	Schmal-lenberg	Spring: Winter wheat Fall: Winter wheat
9	Luvisols	Loess	Southern and South Western Loess Region	Bad Kreuznach	Spring: Sugar beet Fall: Winter wheat
10	Cambisols (and Dystrict Cambisols)	Basement complex and mesozoic surface layers	Northern low mountain range	Schmal-lenberg	Spring: Rye Fall: Rye
11	Rendzinas (and Calcic Cambisols)	Mesozoic lime stones	Southern Karst Region	Nürnberg	Spring: Winter wheat Fall: Winter wheat
12	Luvisols	Loess	Bavarian Loess Region	Nürnberg	Spring: Maize Fall: Winter wheat
13	Cambisols (and Dystric Cambisols)	Basement complex and mesozoic surface layers	Southern low mountain range	Oberstdorf	Spring: Winter barley Fall: Winter barley

Table 3.9. Soil-Climate Scenarios for Italy.

Italy					
No	**Soil type**	**Organic Matter (% OM)**	**Groundwater level**	**Climate Station**	**Representa-tive Crops**
1	Clay	1.24	2.0 m	European scenario No 10: North Italy	Maize
2	Clay	1	no data (1.0 m)	European scenario No 11: South Italy	Wheat

Table 3.10. Soil-Climate Scenarios for The Netherlands.

The Netherlands					
No	**Soil type**	**Organic Matter (% OM)**	**Groundwater level**	**Climate Station**	**Representative Crops**
1	Sand	<3	1.0 m	De Bilt (yr=1980)	Maize, Bulbs
2	Sand	3-6	0.8 m	De Bilt (yr=1980)	Beets, Grains
3	Peat	>6	0.85 m	De Bilt (yr=1980)	Grains
4	Loam	<3	no data (1 m)	De Bilt (yr=1980)	Maize
5	Clay	<3	0.9 m	De Bilt (yr=1980)	Beets, Potatoes, Grains
6	Clay	3-6	0.8 m	De Bilt (yr=1980)	Beets, Potatoes, Grains
7	Clay	>6	0.9 m	De Bilt (yr=1980)	Beets, Potatoes, Grains

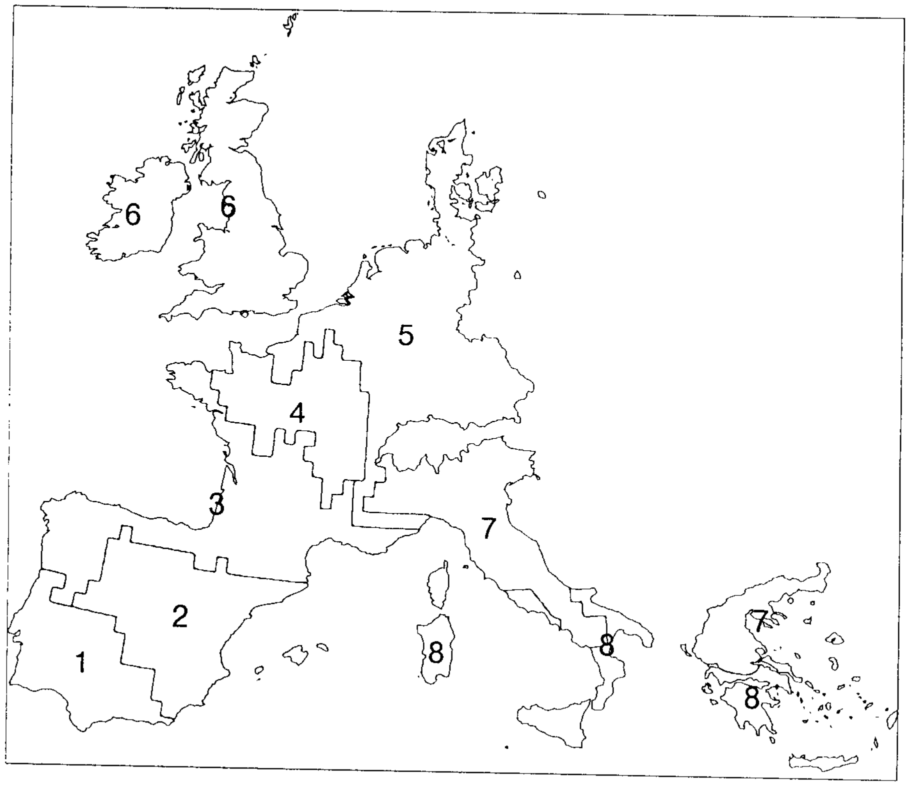


Figure 3.6. Soil-Climate Scenario Map Europe.

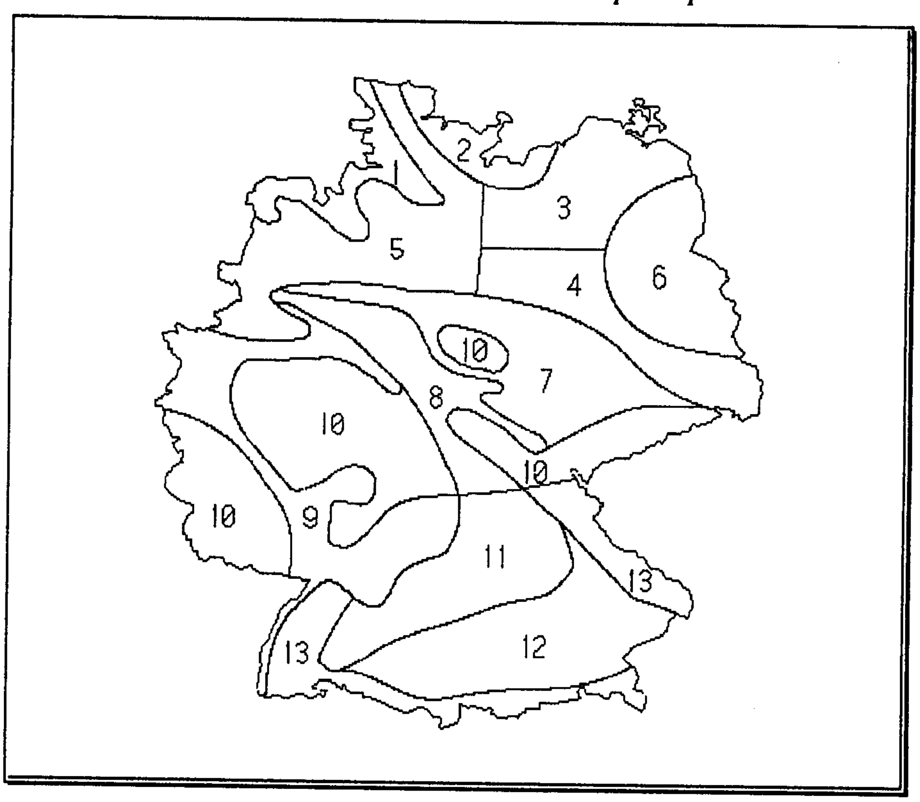


Figure 3.7. Soil-Climate Scenario Map Germany.

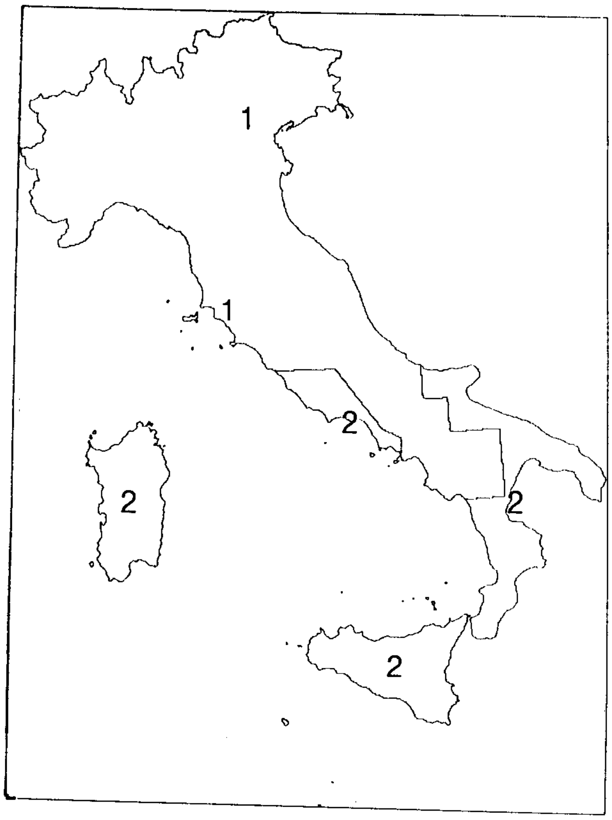


Figure 3.8 Soil-Climate Scenario Map Italy.

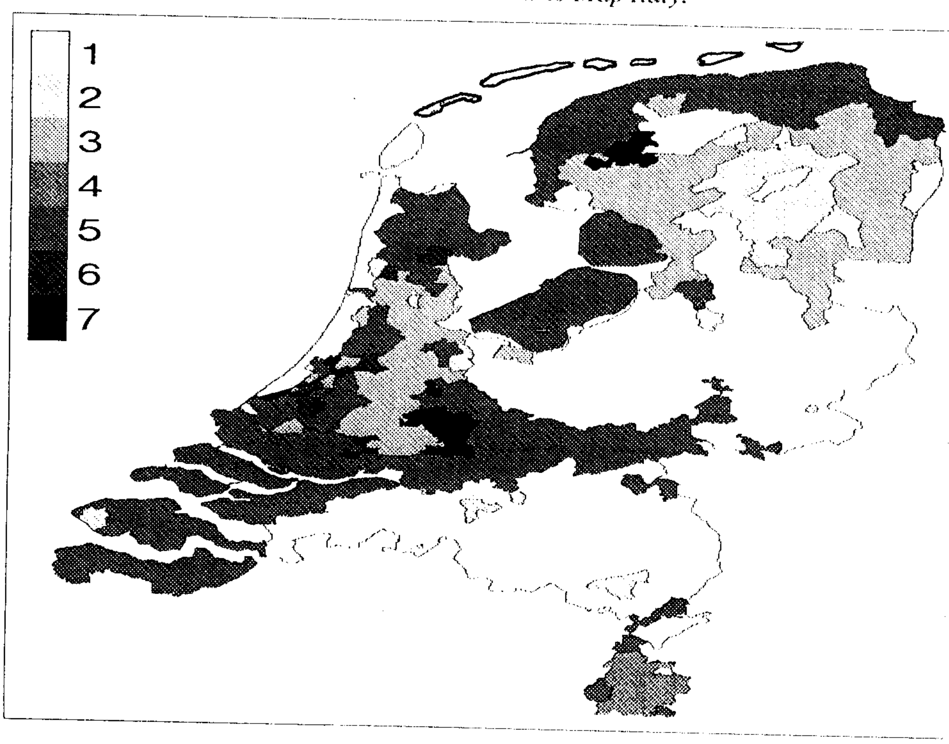


Figure 3.9 Soil Scenario Map The Netherlands.

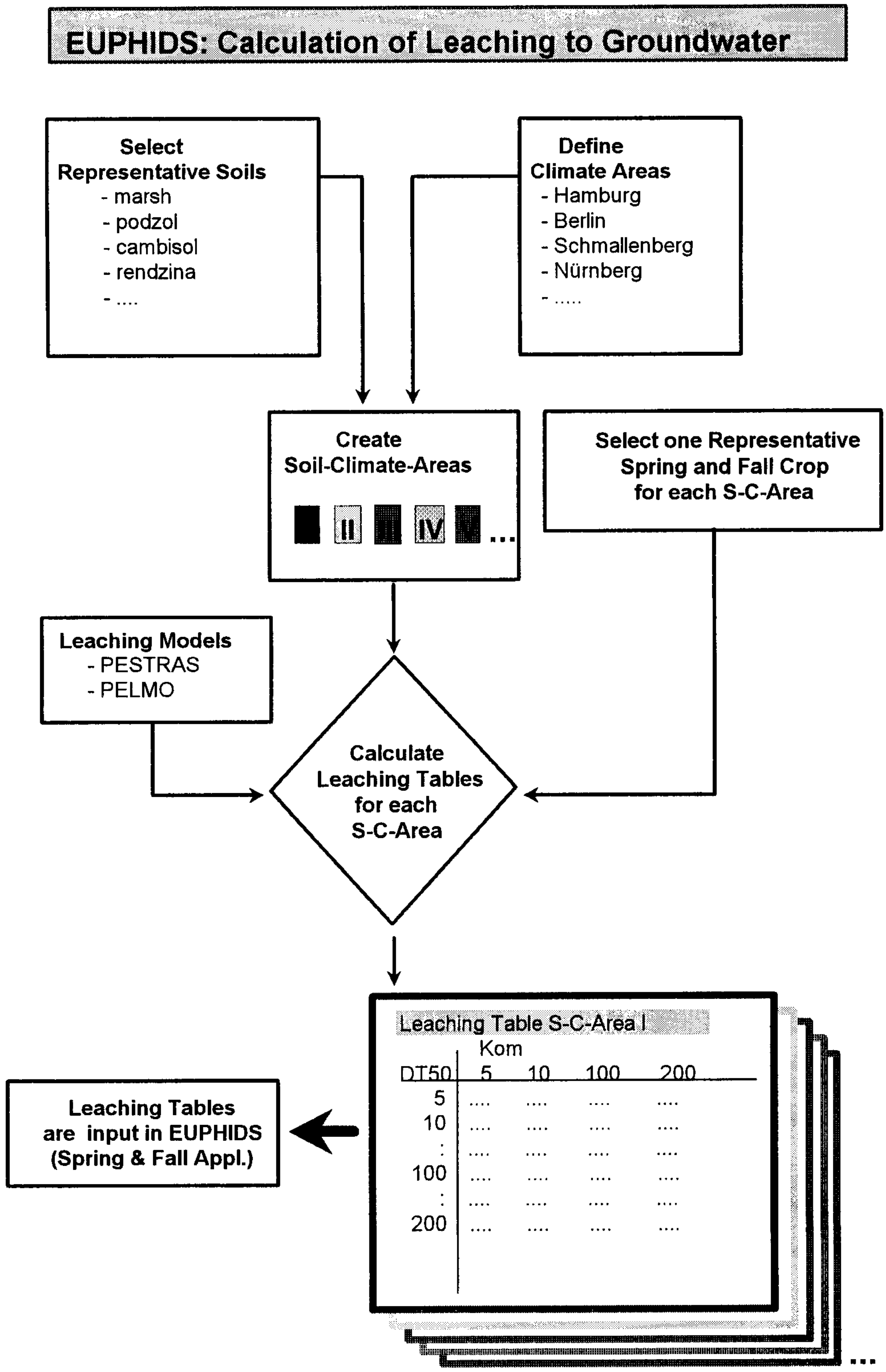
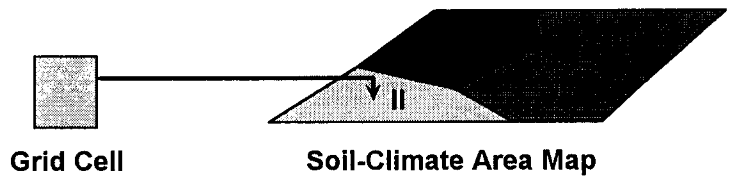


Figure 3.10. The calculation of leaching tables (example for German soils and climates)

EUPHIDS: Calculation of Leaching to Groundwater



Computation in EUPHIDS Leaching Module

- Identify S-C-Area in which Grid Cell is located
- Select respective Leaching Table
- Calculate apparent Kom* for the Pesticide

$$\text{Kom*} = \text{Kom}\,\frac{\%\ \text{OM Grid Cell}}{\%\ \text{OM Reference Soil}} \qquad \text{(OM map)}$$

- Read DT50 of Pesticide
- Compute Leaching to Groundwater by Linear Interpolation in the DT50 - Kom Leaching Table. Use Kom*.

Leaching Table S-C-Area II

	Kom			
DT50	5	10	100	200
5	....	....	....	....
10	....	....	....	....
:	....	....	....	....
100	....	....	....	....
:	....	....	....	....
200	....	....	....	....

- Correct for Dose in order to get PEC Grid Cell

Generate PEC map for Groundwater

Figure 3.11. The calculation of PEC groundwater.

3.3. Evaluation of Pesticide Effects

3.3.1. Types of evaluation

The evaluation of the effects on the environment requires the consideration of different targets and the analysis of several potential risks. EUPHIDS distinguishes between three main types of evaluations:

1. Evaluation of effects on single species.
2. Evaluation of effects on multiple species and ecosystems.
3. Evaluation of effects on multiple compartments.

These three levels can be seen as an evaluations sequence which aim at generating increasingly aggregated figures. The first two type of analyses are also called *threshold analyses* since they aim at evaluating the risk by comparing exposure levels to acceptable levels. The third evaluation, carried out with value functions, is also called *overall evaluation* as it aims at an overall indication of environmental risks.

The evaluation of effects on single species requires the knowledge of the probable exposure of individual species and evaluates the degree to which they are at risk. The Uniform Principles require this type of evaluation. The evaluation of effects on ecosystems aims at gathering information on the degree to which ecosystems as a whole are exposed to risk, beyond the indications given by the risks on individual organisms or species. Finally, the evaluation of effects on multiple compartments aims at integrating effects on soil and water into a risk figure which indicates the degree to which the pesticide affects the environment as a whole.

Probable pesticide risks are evaluated for each single grid cell by comparing PECs for surface water, top soil and groundwater with the respective (no-)effect level data ((N)EL). The basis for the risk evaluation is the (no-)effect level data based on results of standardised and officially adopted single species tests or the groundwater reference value for pesticides (0.1 µg/l). (N)EL data may be:

- single species effect data like LD_{50} and EC_{50} values;
- no-effect data like NOECs or NOELs ;
- no effect levels for ecosystems (e.g. PNEC, HC_5^{50}) obtained by the extrapolation methods as described in the following subparagraphs.

The ecotoxicological risk is estimated from the quotient:

$$\text{Risk} = Q > \frac{\text{PEC}}{\text{(N)EL}} \quad (\Rightarrow \text{for a species or an ecosystem}) \tag{3.26}$$

The quotient Q is used as an indicator of risk. The output of the ecotoxicological risk assessments can be displayed as risk maps.

3.3.2. Evaluation of risks for single species: the Uniform Principles

This option offers the opportunity to create and to compare PEC/(N)EL maps for individual species. The (N)ELs are the results of toxicity tests which are either transformed by assignment of safety factors (UP) or taking the actual levels obtained from toxicity experiments. EUPHIDS offers two possibilities:

1. calculation of the risk quotients following the Uniform Principles;
2. calculation of the risk quotients following the actual ecotoxicological endpoints.

Risk assessment according to the "Uniform Principles" requires the computation of a Q level for a given species with specific (N)ELs. The relevant species for the evaluation of risk to top soil and aquatic ecosystems as mentioned in the Council-Directive 94/43/EC (1994) and are given in Table 3.11. The risk-quotients not to be exceeded are differentiated with respect to the test type (short or long term) and the end points considered (NOECs or effect concentrations). For groundwater, no quotient but the EU-reference value of 0.1 µg/l is given.

Unless the risk quotient resulting from the division PEC/(N)EL does not exceed the prescribed Q levels, it is assumed that no significant environmental effects due to the use of the assessed pesticide will occur. Therefore, the environmental risk of the pesticide is considered as negligible. When a risk quotient exceeds the figure given in the directive no authorisation shall be granted unless it is clearly established through an appropriate risk assessment that under field conditions no unacceptable effects will occur[9].

Table 3.11. Risk-Quotients not to be exceeded according to the "Uniform Principles" (ST=short term; LT=long term).

Environmental Compartment	PEC / (N)EL	Risk-Quotient (Q)
Top Soil		
Earthworms	PEC_{st}/LC_{50} (ST)	< 0.1
	PEC_{lt}/NOEC (LT)	< 0.2
Groundwater	PEC_{lt} GW (LT)	< 0.1 µg/L
Aquatic Ecosystem		
Fish and Daphnia	PEC_{st}/LC_{50} (ST)	< 0.01
	PEC_{lt}/NOEC (LT)	< 0.1
Algae	PEC_{st}/EC_{50} (ST)	< 0.1

EUPHIDS offers an additional options for computing risk quotients. In order to provide the user with indications of risks based on the real ecotoxicological end-points, all the Q levels may be set to one, thus computing risk quotients on the basis of actual NOEC or LC_{50} values.

[9] In the Uniform Principles some more species, risk quotients or maximum values (e.g. for degradation in soil or bioaccumulation in fish) than those considered in EUPHIDS are given. These are not included since they currently cannot be modelled spatially variable (e.g. depression of microbial activity in soil upon pesticide use, bioaccumulation in fish, risk for honey bees and beneficial arthropods) and therefore can simply be checked for compliance with the standards of the "Uniform Principles" by manual comparison of these few figures with the respective standards.

3.3.3. Evaluation of risks for ecosystems[10]

Beside the evaluation of individual organisms/species, EUPHIDS offers the possibility of extrapolating the information on single species to ecosystems and thus to offer a more aggregated risk figure. EUPHIDS implements three methods for computing the ecosystem (N)EL:

1. the EPA method;
2. the safety factors method;
3. the sensitivity distribution method.

If ecotoxicological risk is assessed according to the EPA-Method (EPA, 1984), empirical assessment factors depending on quality and quantity of available tests are assigned to the test result of the most susceptible species in a data set (Table 3.12). The assignment of assessment factors is done to compensate for uncertainty due to the lack of knowledge in terms of variability and possible combinations of ecological and toxicological parameters.

Table 3.12. Assessment factors according to the EPA-Method. (Taxonomic groups are, e.g., fish, crustaceans, algae, earthworms, birds, mammals etc.).

Data Basis	Assessment Factor
acute values for species of less than 3 different taxonomic groups	0.001
acute values for species of at least 3 different taxonomic groups	0.01
NOEC-values for species of less than 3 different taxonomic groups	0.01
NOEC-values for species of at least 3 different taxonomic groups	0.1

The single species test result of the most susceptible organism multiplied by the assessment factor is considered as (N)EL for the ecosystem in which this organism is living. Risk is considered as ratio PEC/(N)EL

$$R = \frac{PEC}{(N)EL} \geq 1 \qquad (3.27)$$

The safety factors option offers basically the same procedure and functionality compared to the EPA-method except that the user has the opportunity to set the safety factors.

[10] Terrestrial ecosystems are currently not considered explicitly in EUPHIDS. This is mainly due to the fact that all terrestrial species which have to be tested for pesticide risk assessment according to the Uniform Principles (Council-Directive 94/43/EC), e.g. birds, mammals, earthworms, and honey-bees, must already suffer no harm upon living on a treated field. Thus, as long as no further ecotox-tests with a broader and more representative spectrum of terrestrial organisms have to be delivered by the applicants or more stringent safety margins for ecosystems than for the treated field are defined, it seems not very meaningful for the purpose of pesticide risk assessment to additionally consider the terrestrial environment as an entity of its own. It is therefore proposed to substitute the assessment of risk for terrestrial ecosystems by the assessment of risk for terrestrial organisms living on a treated field. To be able to conduct the respective risk estimates, appropriate field-scenarios for the calculation of PECs and pesticide uptake of species have already been established but still have to be included in the EUPHIDS system. For more information see the Appendix A7 "Estimation of PECs and pesticide risks for organisms of the terrestrial environment"

Thus, this option offers a flexible evaluative tool that can be adjusted to specific requirements.

As a further option, the environmental risk of pesticides may be assessed by the Sensitivity Distribution method (Kooijman, 1987; van Straalen & Denneman, 1989; Aldenberg & Slob, 1993). Basic assumptions underlying the method are:

1. the sensitivity of the species of an ecosystem to a pesticide can be described as a log-logistic distribution curve and
2. the structure and function of an ecosystem can be protected when 95 % of the species inhabiting this ecosystem are protected from adverse effects.

The Sensitivity Distribution method allows to derive hazardous concentrations of toxic substances from experimental NOECs for the remaining 5 % of the species. The so-called Aldenberg and Slob method (see reference above) accounts for uncertainty in the estimates by calculating the one-sided 50% or 95% left confidence limits from the mean and the standard deviation of a log-logistic distribution based on NOECs of at least 4 tests (Figure 3.12).

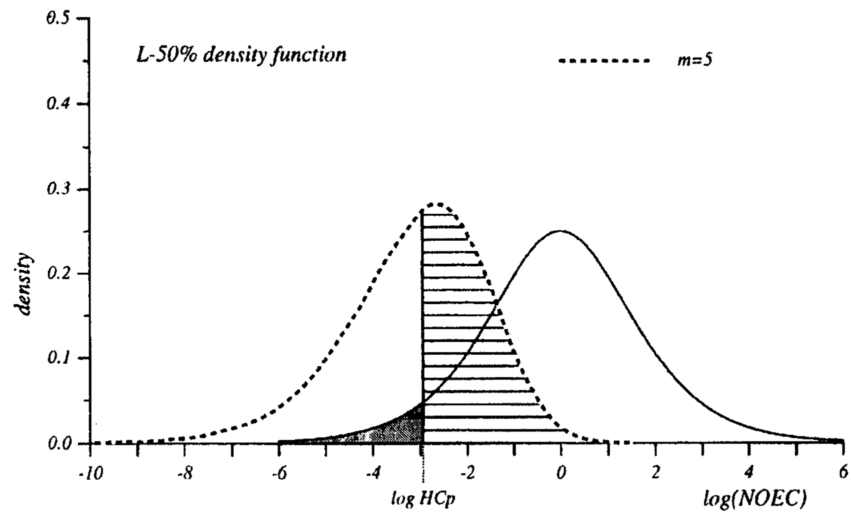


Figure 3.12. Log-logistic sensitivity distribution function for the species of an ecosystem (sample: m = 5). The Hazardous Concentration for 5 % of the species is shaded (log HC_5 = primary risk). The probability density function for the log HC_5 is dashed. The hatched region depicts the secondary risk of over-prediction and thereby harming a larger fraction of species in case of a 50% confidence estimate for the HC_5 (figure from Aldenberg & Slob, 1993).

These tests must be a representative sample for the species of the ecosystem. The consideration of uncertainty is achieved by including an extrapolation constant K_e in the formula used to calculate the hazardous concentrations. This constant K_e is dependent on the number of NOECs of the sample. K_e for different sample sizes was derived by Monte-Carlo simulations (Aldenberg & Slob, 1993).

$$\log HC_5^K = X_m - K_e * S \qquad (3.28)$$

In which:

HC_5^K = Hazardous concentration for 5% of the species of the ecosystem with a confidence of K% (50 or 95%)

X_m = Sample mean

S = Standard deviation of the sample

K_e = Extrapolation constant which is dependent on the number of NOECs of the sample. K_e is read from a table included in EUPHIDS

The risk then is assessed as ratio:

$$R = \frac{PEC}{HC_5^k} \geq 1 \qquad (3.29)$$

3.3.4. Overall evaluation with value functions

The basic form of risk evaluation introduced above requires the comparison of a PEC level with a reference threshold level. This evaluation may be insufficient for two reasons (Fischhoff, 1984):

1. It separates neatly acceptable from unacceptable situations and does not allow for measures of risk intensity (distinctions between PECs far below-above the thresholds and PECs just below-above the thresholds).
2. It does not support the evaluation of simultaneous risks to multiple compartments.

The overall evaluation in EUPHIDS aims at overcoming these difficulties. Within each compartment (top soil, surface water, groundwater) the step-wise separation between acceptable (below the threshold) and unacceptable (above the threshold) level can be improved by introducing intermediate degrees of acceptability. This analysis is called value analysis (Beinat, 1995; Keeney, 1992; Keeney and Raiffa, 1976) and is performed using value functions. The value function method requires a function which attaches to each PEC level a degree of acceptability, usually expressed between 1 (PEC is totally acceptable) and 0 (the PEC is totally unacceptable). Once this is available, the evaluation of the overall risks to the environment is based on a weighted combination of acceptability scores across environmental compartments.

In line with the other evaluation, the overall evaluation scheme based on value functions distinguishes between short term and long term aspects. EUPHIDS considers the overall evaluation to several compartments. Table 3.13 shows, for each compartment, the information necessary for the overall evaluation and the ecotoxicological endpoints used.

For each compartment, EUPHIDS requires the selection of a low-limit threshold (called L) and a high-limit threshold (called H). L indicates levels below which there is evidence of no adverse effects to the target ecosystems (terrestrial ecosystems for the top soil map; aquatic ecosystems for the surface water map). H indicates levels above which there is evidence of unacceptable adverse effects to the ecosystems[11]. The overall risk index depends on the configuration of PEC level between the L and H. Figure 3.13 displays five different grid cells which show different PEC configurations normalised against the corresponding L and H levels.

Table 3.13. Compartments, information and toxicological endpoints for the overall evaluation.

Time	Compartments	Information	Toxicological end points
Short term	- surface water	- surface water PEC map	- (N)EL aquatic ecosystems
	- top soil	- top soil PEC map	- (N)EL terrestrial ecosystems
Long term	- surface water	- surface water PEC map	- (N)EL aquatic ecosystems
	- top soil	- top soil PEC map	- (N)EL terrestrial ecosystems
	- groundwater	- groundwater PEC map	- EU threshold

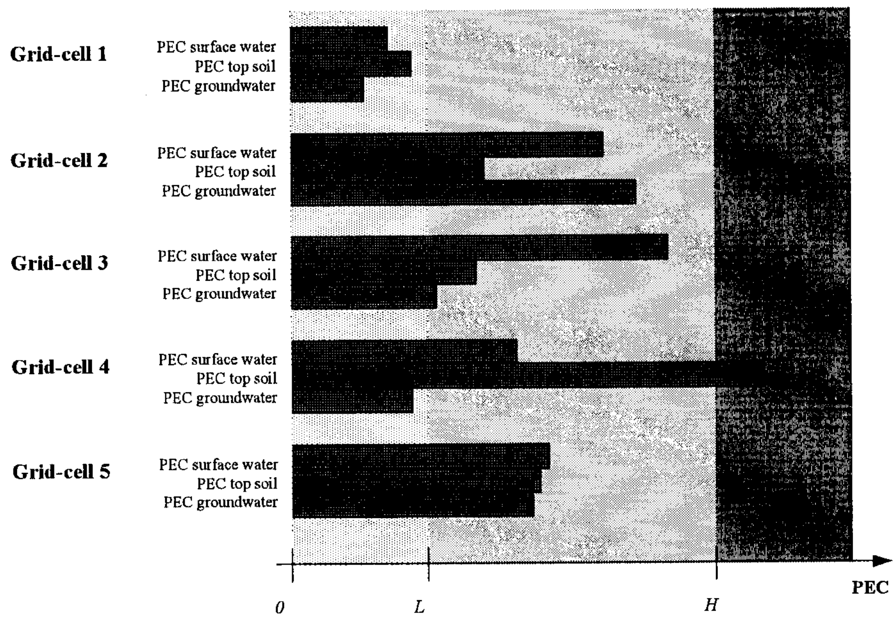


Figure 3.13. PEC levels for five hypothetical grid-cells.

The area in which all grid-cell PECs are below their L (light dotted area on the left) corresponds to the absence of environmental risks for the pesticide (grid-cell 1). The area in which at least one grid-cell is above its H level (heavy dotted area on the right) highlights high risk for at least one compartment, which may lead to a restricted use of the pesticide or to the decision to ban the substance altogether (grid-cell 4). In the other cases, PECs exceeds the L level but within the limit posed by H. Grid cells included in this area show conflicting situations (grid-cell 2, 3 and 5). Their actual evaluation requires to balance out the risks which occur in different compartments.

[11] The thresholds L and H for each compartment are selected on the basis of ecotoxicological tests and expert judgement (cf. the Appendix) and are the same within each map.

The collection of PEC levels of all compartments for each grid-cell represents the risk profile of the grid-cell. The best risk profile (BRP) is defined as the collection of L levels for all compartments; the worst risk profile (WRP) as the collection of H levels for all compartments (Figure 3.14).

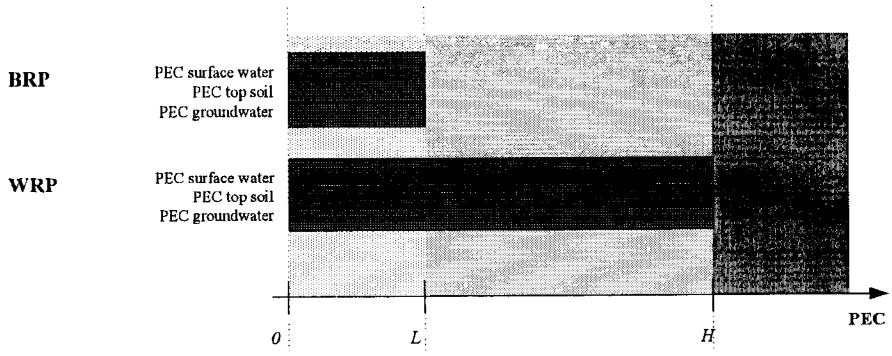


Figure 3.14. Best and worst risk profiles.

The role of value functions is that of processing, for each grid cell, the risk profile and attaching to it a value between 0 and 1. Therefore, a value function v is such that:

$$0 \leq v(PEC_{SW}, PEC_{GW}, PEC_{TS}) \leq 1 \qquad (3.30)$$

where:
PEC_{sw} = PEC surface water;
PEC_{GW} = PEC groundwater;
PEC_{TS} = PEC top soil.

The construction of a value function requires the following steps (Beinat et al., 1994; Fischer, 1977):

1. For each compartment, select the L and H level. A possible selection is L=(N)EL and H=10*(N)EL[12], where (N)EL is the ecosystems (N)EL computed with one of the methods presented above (EPA, safety factors or sensitivity distribution);
2. For each compartment separately, assess a unidimensional individual value function which translates a PEC into a value score between 0 and 1 as follows:

$$v_{SW}((N)EL_{SW})=1 \leq v_{SW}(PEC_{SW}) \leq v_{SW}(10*(N)EL_{SW})=0 \qquad (3.31)$$
$$v_{TS}((N)EL_{TS})=1 \leq v_{TS}(PEC_{TS}) \leq v_{TS}(10*(N)EL_{TS})=0 \qquad (3.32)$$
$$v_{GW}((N)EL_{GW})=1 \leq v_{GW}(PEC_{GW}) \leq v_{GW}(10*(N)EL_{GW})=0 \qquad (3.33)$$

   Thus, the value of 0 is attached to PEC=H, and the value of 1 to PEC=L for each compartment. An example of value functions is given in Figure 3.15.

[12] Levels different than (N)EL and 10*(N)EL for describing the best and worst profile respectively can be used. This selection is justified in the Appendix A2.

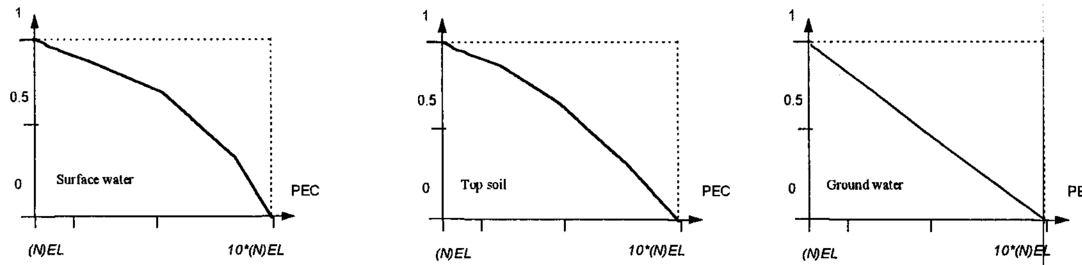


Figure 3.15. Value functions for aquatic and terrestrial ecosystems.

3. For all compartments, select a weight which represents the importance of limiting adverse effects in the compartments in comparison to the other compartments. Weights are indicated with w_{SW}, w_{TS}, w_{GW}.
4. Combine individual value functions with weights and determine the overall value function[13]. The additive multicriteria value function is computed as:

$$v(PEC_{SW}, PEC_{TE}, PEC_{GW}) = w_{SW} * v_{SW}(PEC_{SW}) + w_{TE} * v_{TE}(PEC_{TE}) + w_{GW} * v_{GW}(PEC_{GW}) \quad (3.34)$$

where the values of 0 and 1 correspond to:

$$v(L_{SW}, L_{TS}, L_{GW}) = v((N)EL_{SW}, (N)EL_{TE}, (N)EL_{GW}) = 1 \quad (3.35)$$

$$v(H_{SW}, H_{TS}, H_{GW}) = v(10*(N)EL_{SW}, 10*(N)EL_{TE}, 10*(N)EL_{GW}) = 0 \quad (3.36)$$

Figure 3.16 shows the results of the application of a value function to the grid cells in Figure 3.13, when each compartment is assigned an equal weight.

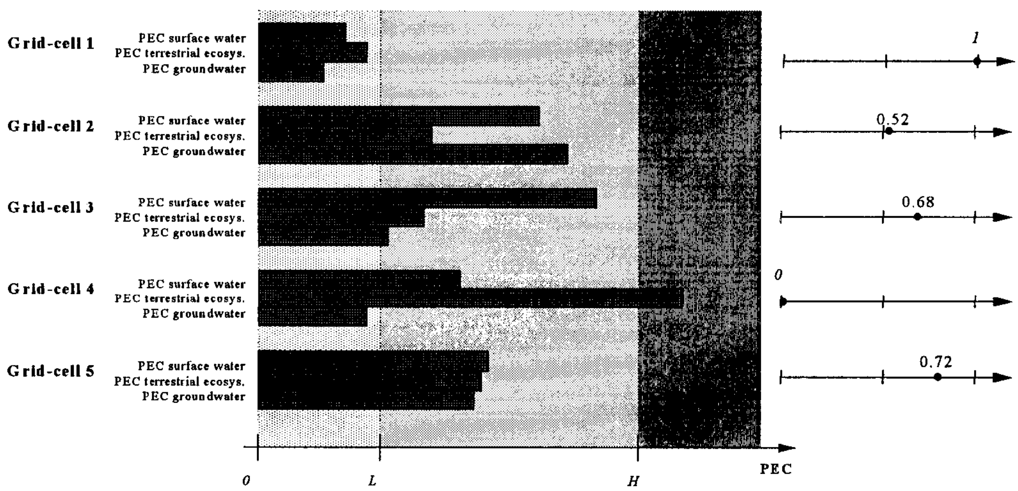


Figure 3.16. Overall values attached to the grid cells.

[13] This scheme assumes compensation across categories within L and H (Bouyssou, 1986). For instance, a small increase in surface water PEC can be balanced by an appropriate decrease in top soil PEC. Compensation means only that, in global terms, the situation is as acceptable (or unacceptable) as before. Compensation does not imply any kind of physical compensation mechanism among effects on different species.

The result of the overall evaluation with value functions is an overall risk map. This map shows, for each grid cell, a risk index between 1 and 0. This value depends on all the risks of all the compartments introduced in the evaluation and gives an overall picture of the risk to the environment. There are several techniques which can be used to assess value functions and weights. Appendix A2 shows some basic ideas for this purpose. A complete description of techniques for assessing value functions can be found in Beinat (1995).

3.4. Spatial evaluation

Spatial evaluation deals with the spatial distribution of environmental risks. It aims at capturing the relevant insight in the spatial patterns and regularities of risk distribution. EUPHIDS allows the analysis of spatial distribution for input and output maps. The system offers the following possibilities: map statistics; map filtering; map uncertainty and map aggregation. The map shown in Figure 3.17 will be used along the exposition to illustrate the various options.

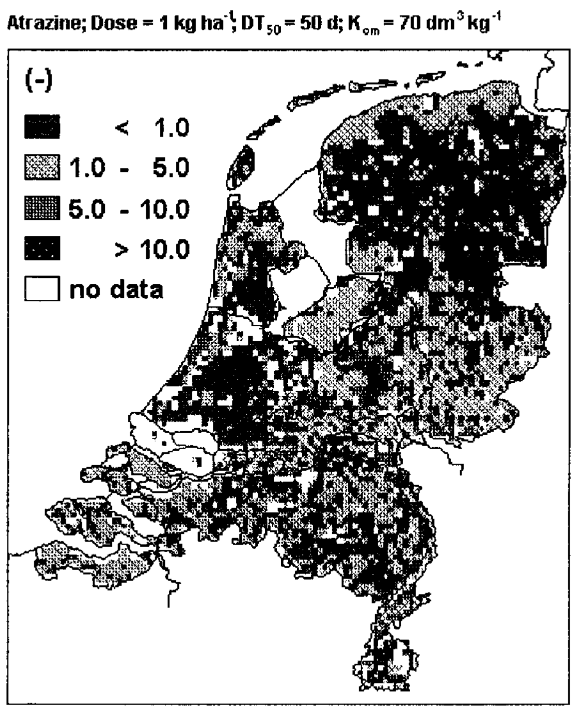


Figure 3.17. Example map with four classes: risk ratios PEC/reference for atrazine leaching in groundwater in the Netherlands.

3.4.1. Map statistics

Map statistics calculate the map distribution of grid-cells into classes. EUPHIDS allows three types of statistics:

1. map classification;
2. reclassification;
3. cumulative distributions.

An example of map classification is shown in Figure 3.18. Map classification counts the number of grid-cells within each class and offers a numerical synthesis of the map content. The classes boundaries are pre-defined in EUPHIDS.

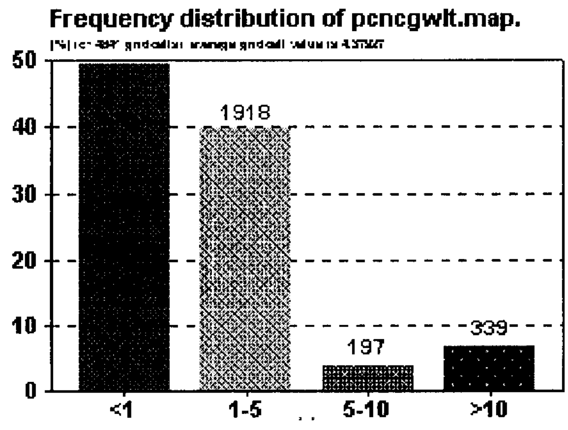


Figure 3.18. Example of map statistics for the map in Figure 3.17. The average of the grid cells is 4.38.

Map reclassification uses the actual data in the map to specify the classes. EUPHIDS first reads the minimum and maximum value in a map and then divides the interval in the same number of classes used for map classification. The resulting histogram shows the actual numerical distribution of grid cell values between the minimum and maximum value. A similar information i provided by the cumulative distribution. This options show the cumulative cell distribution starting from lowest to the highest values found in the map.

Map statistics are mainly used for a numerical of the map content. It processes spatial information into numerical information, which is easier to read and interpret. However, the spatial content of information is lost. Map statistics are also useful when decision rules are stated in terms of spatial frequency or cumulative distributions. For instance, a decision rule could the following. The pesticide can be admitted if:

- the PEC exceeds the (N)EL in no more than 5% of the area;
- PEC never exceeds 2*(N)EL .

This decision rule can be verified directly through an appropriate map statistics.

3.4.2. Map filtering

Map filtering reduces the map variability and enhances the clarity of trends and patterns. The values of the map are smoothed out taking into account the neighbour cells. Each grid-cell is assigned a new value which depends on its current value and on the surrounding values. Figure 3.20 shows an example in which each grid cell score is the average of its original score and of the eight surrounding cells. The result is a simpler map showing uniform areas and patterns more clearly.

Map filtering requires two types of information:

1. a map classified into a finite number of classes;
2. the filtering lag.

The filtering mechanism is shown graphically in Figure 3.19. The value attached to the filtered map is the average of the values of the corresponding grid-cell in the original map plus the values of the surrounding cells within the lag specified. Grids for which no values are available are disregarded.

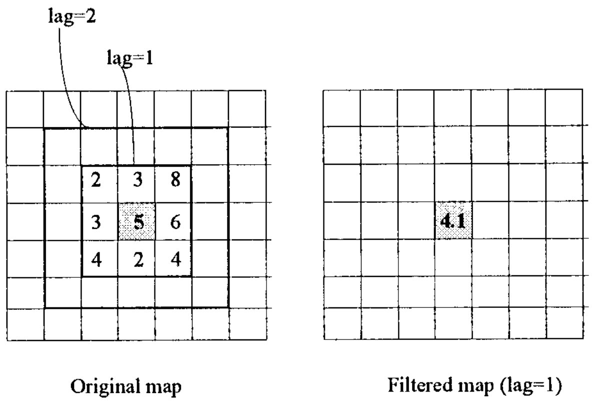


Figure 3.19. The filtering mechanism.

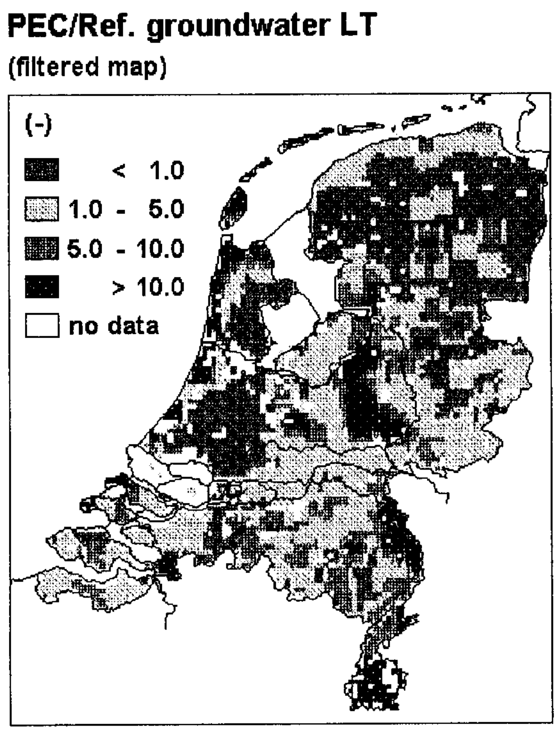


Figure 3.20. Map filtering applied to the map in Figure 3.17.

The filtering lag determines the number of grid cells to be taken into account. If the lag is 1, then the filtered map attaches to each grid cell the average of its original value and of the 8 surrounding cells; if the lag is 2, then the surrounding cells become 24 and so on and so forth.

Map filtering is used to isolate uniform areas in a map. Its usage becomes particularly effective when admission policies can be spatially differentiated, for instance through limitations on the use in certain areas. The result of map filtering gives an indication of the size in which different policies may be applied. It also serves for a comparison of the administrative boundaries in which these policies can be implemented and the environmental boundaries in which they are effective or required. Map filtering can also be applied to noise removal. By smoothing out the map content random data error is smoothed increasing the reliability of the map.

3.4.3. Map uncertainty

Most map analyses rely on data classification. Uncertainties in original data, in modelling environmental aspects and in selecting the classification schemes are responsible for classification sensitivity. Due to uncertainty in the information used for the computation of the PEC or for the assessment of the (N)EL, some grid cells might have an uncertain classification. Correspondingly, for each grid cell it is necessary to accommodate for an additional class, called uncertainty class, which includes cells which classification changes due to data uncertainty. The amount and distribution of uncertainty is a measure of the reliability and robustness of results against uncertainty.

Uncertainty analysis in EUPHIDS is based on the analysis of the effects of uncertainty on a single threshold. Multiple analysis may thus be required to test the robustness of the results against different threshold values.

The analysis requires three types of information:
1. a PEC map to be analysed;
2. the threshold for which classification uncertainty has to be calculated (T);
3. the uncertainty fraction (F).

For each grid cell, the classification is the following:
1. if $PEC - F \cdot PEC > T$, then the cell is classified above the threshold;
2. if $PEC + F \cdot PEC < T$, then the cell is classified below the threshold;
3. otherwise, the cell is classified as uncertain.

Figure 3.21 shows the result of map uncertainty applied to the 0.1 μg/l threshold for groundwater PECs. The uncertainty fraction is set at 0.8. The uncertainty class shows grid cells that may take on a PEC higher or lower than the threshold due to the uncertainty fraction applied.

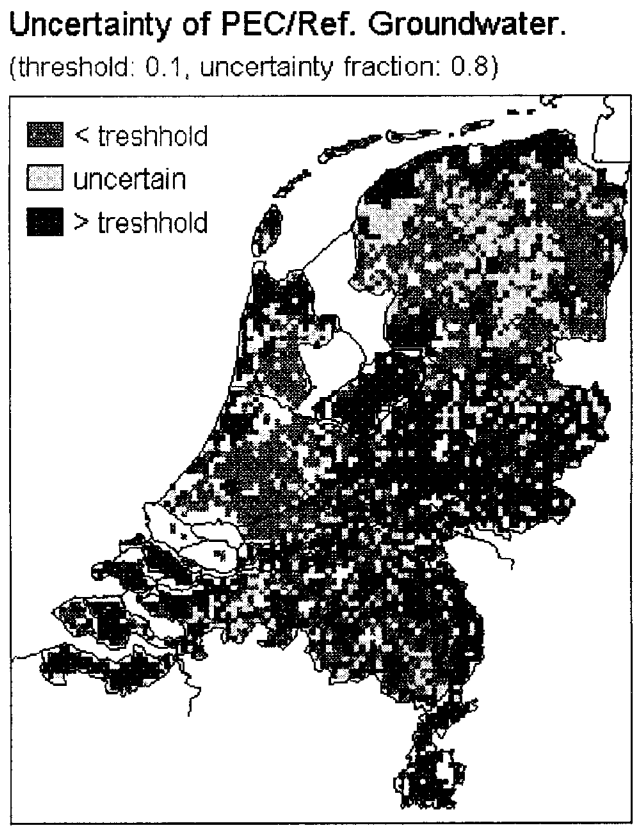


Figure 3.21. Map uncertainty for the PEC groundwater map. The uncertainty is calculated against the 0.1 µg/l threshold.

3.4.4. Map aggregation

The input and output maps in EUPHIDS are represented in a special type of spatial entities: the grid-cells. Map aggregation aims at offering a different representation based on other types of spatial entities, for instance municipalities, provinces etc.. Map aggregation requires three types of information:

1. the map to be aggregated;
2. the type of spatial entities to aggregate into;
3. the aggregation rule.

EUPHIDS offers the aggregation into two types of spatial entities: regions and land use. Within each selected entity (for instance, provinces) the original PEC levels are aggregated using one of the following aggregation rules:

1. Average. The aggregated value is the average of all grid cells values within the spatial entities selected. Figure 3.22 shows the aggregated map for groundwater risks. The risk ratio attached to each province is the average of the risk ratios of all the grid-cells within the province boundaries.
2. Maximum. The aggregated value takes on the maximum value between all grid cells within the entities selected.
3. Threshold exceedence. The aggregated value is the number of grid cells within the selected entities which exceed a threshold specified by the user.

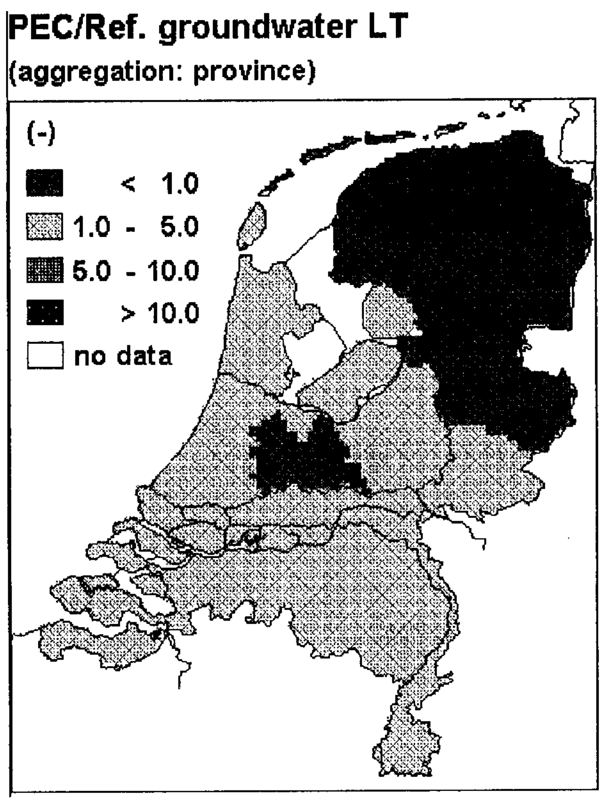


Figure 3.22. Spatial aggregation: aggregation of groundwater PEC/reference (average aggregation) a the level of provinces in the Netherlands.

4. Methods for the assessment of human health risks: general population and agricultural workers

4.1. *Assessment of human exposure*

4.1.1. Introduction

The toxicological evaluation of the potential risk of pesticides to human health is an essential component of a Decision Support System (DSS) for pesticide registration. Ideally humans should never experience adverse effect of pesticides; however, this ideal situation is very difficult to achieve because pesticides are inherently toxic substances that are deliberately released into the environment and handled by a great number of subjects. Historically, the risk of toxic effects has been documented under various circumstances. First, occupational over-exposure may take place in production or application as safety precautions may not be perfect or not sufficiently known or practised by the operators. Second, pesticides are effective poisons which can be misused for suicide or homicide. Third, exposure of humans to residues of pesticides may take place every day through air, food and water and, due to the essentiality of these media, concern the entire population. To this respect, it has to be remembered that even rare effects (e.g. with a frequency of 10^{-6}-10^{-7}) may produce a substantial number of events when applied to populations of a very large size. Results from studies in humans exposed occupationally, accidentally, or via play an essential role in risk assessment. Risk assessment in toxicology is a process whereby relevant biological, dose-response and exposure data are combined to produce a qualitative or quantitative estimate of adverse effects from a defined chemical agent.

The key question to be answered for the assessment of risk is "Are predicted exposures safe?". In order to answer this question, two separate evaluations are needed:

1. a detailed evaluation of the toxicity of the compound, and the likelihood of expression of any adverse effects in the human organism; this process ultimately derives a "No Observed Effect Level" (NOEL);
2. an estimation of the exposure level and of the amount of compound absorbed during exposure, through each potential route of absorption.

The characterisation of the risk experienced under the proposed conditions of use can be derived from the two basic processes mentioned above; risk characterisation is ultimately the ratio between the absorbed dose and the NOEL. The assessment the magnitude, route and source of exposure plays a central role in the evaluation of the risk posed by pesticides to human health. The magnitude of human exposure to pesticides ranges from low doses, typical for the general population, to high level exposures for of workers in occupational settings (farmers, applicators and industrial manufacturers). The major exposure of the community takes place is via oral route through residues on food, whereas the main exposure of agricultural workers is via respiratory and dermal routes through residues in air, skin contamination during handling and application, and contact with contaminated surfaces.

4.1.2. Assessment of exposure of the General Population

4.1.2.1. Background

As already mentioned, the General Population is mainly exposed to pesticides through the oral route by ingestion of residues with food and drinking water. Although the use of pesticides and agricultural chemicals benefits food production, the residues remaining on foods pose potential health risks to consumers. The estimation of the actual dietary intake of contaminants, as a measure of exposure, is necessary for the risk assessment process.

Collection of valid data on food consumption habits of a population is the most difficult task to be accomplished in assessing the dietary intake of a contaminant. Patterns of food consumption may vary considerably within individuals and groups of individuals such as:

- ethnic and cultural minority groups within a community;
- infants and young children, the elderly;
- pregnant or lactating women;
- people on restricted diets (low-calorie, low-sodium, vegetarian, etc.)

The food consumption data used to determine the dietary intake of a contaminant for a population group should reflect typical food consumption patterns of the population of concern. In principle, data should be derived from current national food consumption surveys which are acceptable sampling techniques for determining food consumption.

International consensus exists on the methodology to be used for collection of data and prediction of dietary intake of contaminants. Reference documents are "Guidelines for the study of dietary intake of chemical contaminants" of the Joint UNEP/FAO/WHO, GEMS, 1985 and "Guidelines for predicting dietary intake of pesticide residues" of the Joint UNEP/FAO/WHO Food Contamination Monitoring Programme in collaboration with the Codex Committee on Pesticide Residues, 1989.

Exposure (based on estimated or measured data) should be compared with the acceptable daily intake (ADI), a milestone concept in toxicology. The ADI of a chemical is defined as the daily intake which is expected to be without appreciable risk during an entire lifetime and is expressed in milligrams of the chemical per kilogram of body weight (mg/kg). For this purpose "without appreciable risk" is defined as the practical certainty that adverse effects will not occur in a lifetime period.

There are several possible indices of food consumption, a commonly used index being the average daily consumption. The three indices of exposure accepted at international level are the following.

Theoretical Maximum Daily Intake (TMDI): estimate of dietary intake (per person), based on the assumption of residue concentrations in the food on the market equal to the maximum limit values (MRL) and average daily per capita consumption of each food commodity (DV) for which an MRL is established. The TMDI is expressed in milligrams of residue per person.

$$TMDI = \sum_{i=1}^{n} MRL_i \times DV_i \qquad (4.1)$$

with:

i = type of agriculture product (e.g. apple, wheat. etc.)

Estimated Maximum Daily Intake (EMDI): this index is a prediction of the maximum daily intake of a pesticide residue based on the assumption of average daily food consumption per person and maximum residues in the Edible Portion (EP) of a commodity, corrected for reduction or increase in residues resulting from preparation, commercial processing and cooking of the commodity (Transformation Process Coefficient, TPC). The EMDI is expressed in milligrams of residue per person.

$$EMDI = \sum_{i=1}^{n} MRL_i \times EP_i \times DV_i \times TPC_i \qquad (4.2)$$

with:

i = type of agriculture product (apple, wheat. etc.)

Estimated Daily Intake (EDI) = estimate of the daily intake of a single pesticide, present as a residue in all foods derived from crops where its use is intended (or admitted in the case of re-registration of pesticides already in the market): it is based on the most realistic estimation of residue levels in the Edible Portion of food and the best available food consumption data for a specific population. It takes also into account the reduction or increase in residues resulting from preparation, commercial processing and cooking of the commodity (TPC), the proportion of the crop treated with the pesticide considered (market share, MS) and the residue concentrations effectively measured in the field with crop and food monitoring campaigns (APR). Since this type of information is usually available at national level, EDI prediction can only be performed at national or regional scale and are useful only to maintain or re-assess registration of pesticides. The EDI is expressed in milligrams of residue per person.

$$EDI = \sum_{i=1}^{n} APR_i \times EP_i \times DV_i \times TPC_i \times MS_i \qquad (4.3)$$

with:

i = type of agriculture product (apple, wheat. etc.)

In order to also evaluate the pesticide residue intake from drinking water, the above indices have been modified as follows:

$*EDI$ = EDI + (Source Water Residue) × (Water Consumption) × (Potability Process Coefficient)

*TMDI = TMDI + (Maximum Residue Concentration in water) × (Water Consumption)
*EMDI = EMDI + (Maximum Residue Concentration in water) ×(Water Consumption)

Thus the variables identified for the estimation of general population exposure are the following:

APR = Agriculture-Produce Residue concentration. This value is necessary for a better prediction of the EDI value at national or regional level. This may vary from country to country for many reasons. Such information can be derived from various sources including supervised trials, survey sampling and analysis and monitoring data.

DV = Diet Values. It is an estimate of the daily average per capita quantity of food or groups of foods consumed by a specific population. This value may change from country to country due to different dietary habits. In order to predict pesticide residue intake at European level, averaged diets need to be developed for a number of dietary patterns representative of the various regions of Europe.

DWC = Drinking Water Consumption. This value may be fixed equal to 2 l/day/person.

EP = Edible Portion. Data on edible portion of commodities are necessary for a more realistic prediction of the pesticide residue intake. In fact, residues that occur on the surface of fruits such as melons, pineapples, bananas and oranges are not consumed since the peel is discarded.

MRL = Maximum Residue Limit. It is defined as the maximum residue concentration of a pesticide residue, resulting from the use of a pesticide according to good agricultural practice, that is intended to be legally permitted or acceptable in or on a food, agricultural commodity or animal feed. MRL are recommended at international level by the Codex Alimentarius Commission for several foods, but may vary from country to country according to different national legislation.

MS = Market Share of the pesticide. This values takes into account the proportion of a crop treated (or likely to be treated) with a particular pesticide.

MRC = Maximum Residue Concentration. This value is currently 0.1 μg/l for drinking water in Europe after the EEC Directive 80/778.

PPC = Potability Process Coefficient. Potability process may influence the concentration of residues in water (for example the active charcoal filtration in potability processes eliminate the presence of pesticide residues in drinking water).

TPC = Transformation Process Coefficient. Many commodities are processed before consumption. These processes may increase or decrease the concentration of residue of pesticide in food. Lipid-soluble pesticides, for example, that concentrate in crude vegetable oil are frequently removed by the refining processes used to make the oil suitable for consumption. These data, when available, lead to a more realistic evaluation of pesticide intake than the TMDI.

SWR = Source Water Residue concentration. These values can be derived from surveys based on sampling and analysis or monitoring data.

Pesticide residue intake through the diet can be predicted with different degrees of accuracy:

1. Crude estimate: TMDI.
   The TMDI overestimates the true pesticide residue intake because:
   - the proportion of a crop treated with a pesticide is usually less than 100%;
   - a minor portion of the treated crop contains the maximum residue level;
   - the concentration of residues in a treated commodity can be modified (usually decreases) during storage, transport, preparation, commercial processing, and cooking;
   - the MRL applies to the whole raw agricultural commodity, which frequently includes inedible portions.

2. Intermediate estimate: EMDI.
   Although EMDI is a more realistic estimate of true pesticide residue intake than TMDI, it is still an overestimate because:
   - the proportion of a crop treated with a pesticide is usually less than 100%;
   - a minor portion of the treated crop contains the maximum residue level;

3. Best estimate: EDI.
   Calculation of EDI is based on data generally available at national level. This evaluation requires adequate information on food consumption, nature and amount of imported food commodities, market share of pesticides, residue concentrations actually present in food commodities.

In estimating both TMDI and EMDI at international level, it is assumed that pesticide residues are present only in commodities for which there are Codex MRLs. Prediction of EDI, usually carried out at national level, requires information on the actual uses of the pesticide on both home-grown and imported foods.

TMDI and EMDI, the less realistic predictions, are relatively easy to carry out but may give a great overestimate of the pesticide intake. However, by starting with the most exaggerated and conservative prediction (TMDI), it is possible to accept, at an early stage, those pesticides whose intake is clearly unlikely to exceed ADI irrespectively of specific data on diet or proportion of use. More realistic prediction, using refined data, are necessary for other pesticides which might exceed the ADI under realistic conditions of use. Therefore, a three-tier approach to predict pesticide residue intake has been proposed.

4.1.2.2. Methodology

The prediction of pesticide residue intake requires two types of information:
1. information related to diet;
2. information related to pesticide residues.

To evaluate the intake with diet of a particular residue it is necessary to identify all crops on which the use of the pesticide is allowed. Pesticide use can be allowed on a class of crop, (leaf-vegetable, for example) or on a particular culture (peas). MRL values are established for a single agricultural product like peas, for a subclass like legumes, for a class like fruit-vegetables, for categories like vegetables or cereals. A residue table has been constructed and it collects information related to the considered pesticide: MRL values allowed on a particular crop; APR values derived from monitoring programmes; TPC values derived from literature or extrapolated from experimental data, chemico-physical characteristics of the pesticide, and type of processing; and MS values. These values are specific for each pesticide. MS and TPC may vary in different areas according to pesticide market and food processing habits. Table 4.1 shows the structure of the residue table.

Table 4.1. Residue table: example extracted from the Italian database.

PESTICIDE	prod_code	MRL (mg/kg)	APR (mg/kg)	TPC	Market share
Pesticide considered	Item or subclass or class or category on which a MRL has been established or an APR has been measured	Maximum residue limit allowed by national law on the product	Agricultural product residue measured on product during survey sampling	Proportion of pesticide remaining on the product after a treatment (boiling, washing)	Proportion of pesticide used on agricultural product (f.i 0.2 of maize is treated with atrazine)
Atrazine	3CAB[1] (cabbage)	0.1	-1[2]	0.4	-1[2]
Methamidophos	3MAI[1] (maize)	0.15	-1[2]	-1[2]	-1[2]
Methamidophos	3PAS[1] (pasta)	-1[1]	0.00036	-1[2]	-1[2]

[1]) Example of code used to identify the item.
[2]) -1 is the identification of a missing value

Diet is characterised by agricultural products (such as apples, peas, rice) and "derived products", that is to say food commodities prepared with the agricultural products (i.e. bread, cakes, pasta). A diet value table has been constructed to collect information characterising a national or regional diet: the average diet values (g/day/person), their standard deviation, the edible portion and the equivalent weight. The equivalent weight is the proportion of a derived product with respect to the original agricultural product (i.e. bread vs. wheat). Table 4.2 shows the structure of the diet table.

A dictionary table, the classification table, relates the two above mentioned tables. This classification is necessary as a pesticide may be allowed (i.e. has a MRL) on a single agricultural product (peas) or on a subclass (legume) or on a class (fruit-vegetables) or on a category (vegetables) while an APR value may be measured also on a derived product like pasta. Table 4.3 shows the characteristics of the classification table.

Table 4.2. Diet table: example extracted from the Italian database .

Food code	Diet (g/day/person)	EP	Equivalent weight	EW-code
Code related to the food item consumed	Mean quantity of the specified food consumed daily by a person	Edible portion of the product	Derived products are expressed as a proportion of the original agricultural product (bread=wheat)[1]	Code of the original agricultural product
3BRE (bread)	158	1	1.13	3WHE (wheat)
3OLO (olive oil)	25.4	1	5	3OLI (olive)
1AUB (aubergine)	7	0.92	1	1AUB

[1]) when the food code identifies an agricultural product, Equivalent weight is equal to 1 and EW-code repeat the food code.
[2]) -1 is the identification of a missing value

Table 4.3. Classification table: example extracted from the Italian database".

Category code	Category description	Class code	Class description	Subclass code	Subclass description	Food item code	Food item description
4CER	cereals	3RIC	rice	NA	not available	NA	not available
4VEG	vegetables	3FVG	fruit vegetable	2SOL	solanaceous	1TOM	tomatoes
4DPR	derived products	3OLO	olive oil	NA	not available	NA	not available

A fourth table is the water database. In this table two types of water source are considered: tap water and bottled water. For the bottled water a Potability Process Coefficient equal to one has been considered on the assumption that, generally, no pesticides are found in bottled water. In Figure 4.1 the flow-chart representing the linkage among the identified variables is shown. As already stated, the flow-chart is divided into two routes: the pesticide and the diet route which are linked in the evaluation of the three indexes of dietary intake. In order to clarify the linkage among the variables, a numeric example has been reported in Figure 4.2: the evaluation of the TMDI, EMDI and EDI for Methamidophos. In this example the group of crops on which an MRL has been established, the disaggregation of these crops in their subclass or item, the relative Transformation Process Coefficients and Edible Portions and, finally, the evaluation of the three indexes are depicted.

Some of the variables identified for the evaluation of the dietary intake are characterised by a geographical (spatial) component:

- DV: data on food consumption are derived from surveys and can be collected at national level or at regional level or at local level;
- APR: data on measured residue level of pesticides in food are collected and evaluated at local and national level;
- MRL: these data are established at national level;
- TPC: these values may vary according to local uses, cultures and habits;
- MS: information can be obtained at national, regional or local level
- SWR: data on surface water residues can generally be collected at local level.

Therefore, the evaluation of dietary intake can be spatially allocated on the basis of the available data. Due to difficulties in obtaining data on APR and SWR, only the spatial allocation of diet values has been considered in developing the module. Therefore, when a country is broken down for regional diets, the output of the module for the General Population is a map showing the different regional exposure assessments. An improvement of this module could be the spatial design of the water database: the tap water-PPC value can vary according to the different sources. The localisation of these sources on the territory together with the specification of values for APR, TPC and MS, could allow a more detailed geographical differentiation of the exposure.

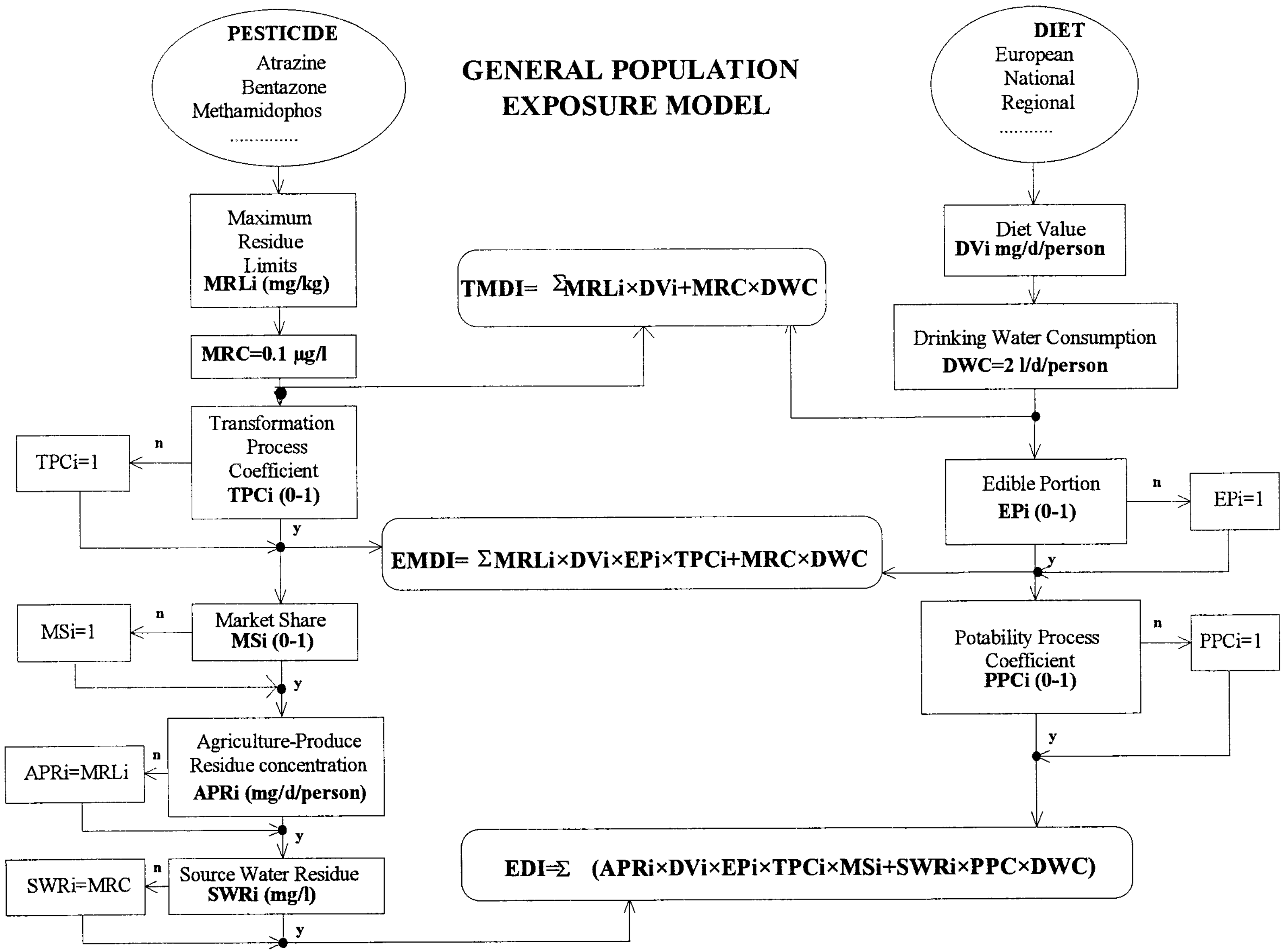


Figure 4.1. General Population Exposure Assessment flow-chart.

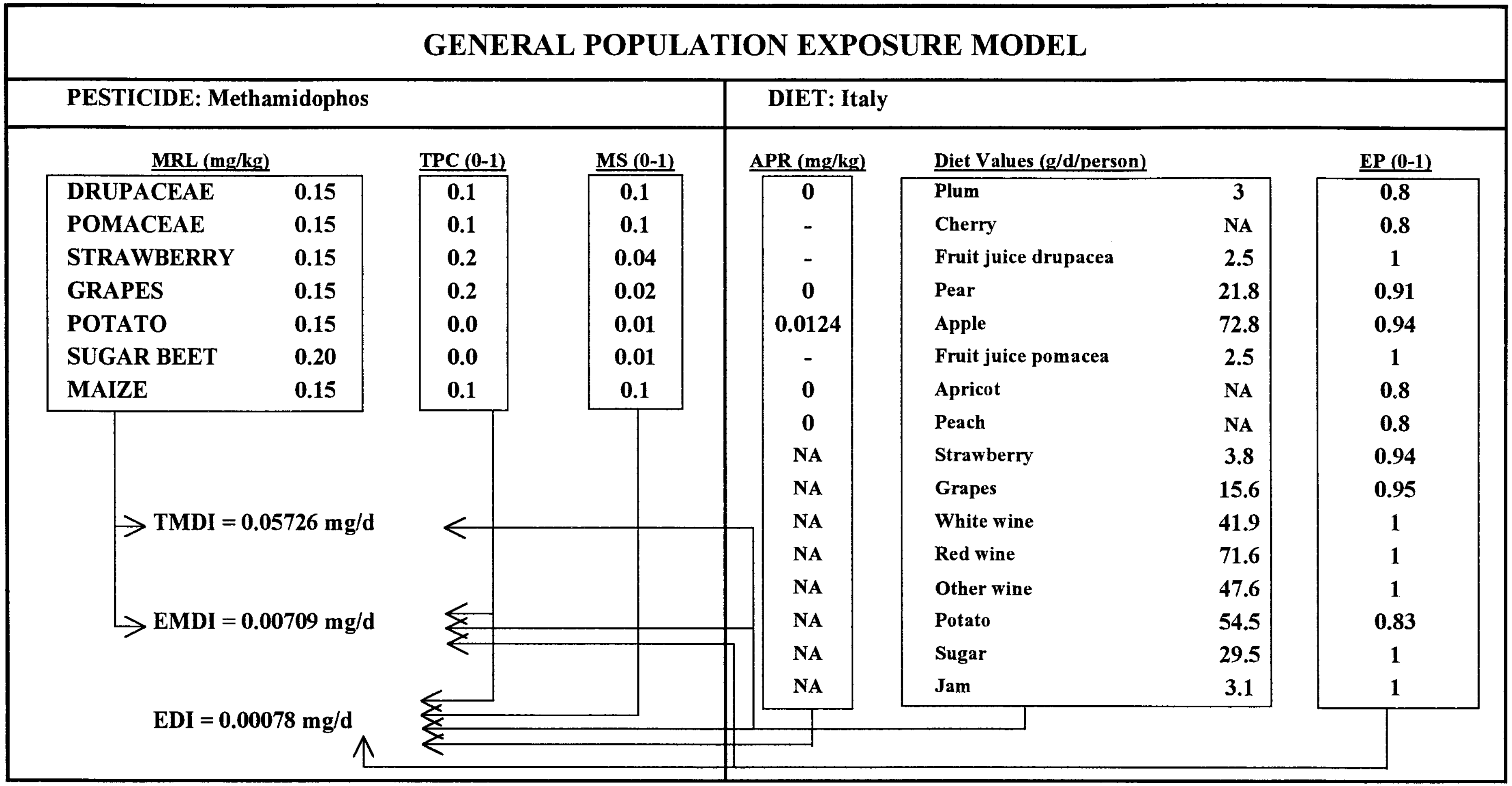


Figure 4.2. Methamidophos: numeric example of the evaluation of TMDI, EMDI, EDI.

4.1.3. Assessment of exposure of Agricultural Workers

4.1.3.1.Background

Subjects with occupational exposure to pesticides include agricultural workers (mixers, loaders, applicators, and harvesters), professional pesticide applicators who treat dwelling, buildings and workplaces, and workers in pesticide manufacturing plants. Occupational exposure to chemicals in agriculture is generally recognised to have the potential for higher doses to the individuals, because of the magnitude and frequency of contact. The number of acute illnesses among agricultural workers is of significant concern to public health authorities. In consideration of the characterisation of exposure and the number of involved subjects, farmers can be considered the most important population group to be protected from pesticide exposure from a public health point of view.

Agricultural workers are exposed to pesticides mainly through the dermal and inhalation routes. Exposure is defined as the amount of a compound (pesticide) available for inhalation, dermal and oral absorption under given ambient conditions. It is denoted external exposure, in contrast to internal exposure, which is the amount absorbed. Many factors may affect the level of exposure and very many variables may be involved in the evaluation of workers' exposure. Moreover the exposure level is strictly related to the handling and applying procedures and practices.

While the toxicity of a new pesticide can be assessed by evaluating data obtained in a series of studies conducted in accordance with well established and internationally agreed guidelines (OECD, 1981), there is no such consensus in respect of the assessment of exposure. As risk assessment necessarily precedes the widescale use of a new pesticide, exposure data specific to the compound under evaluation are usually not available. Consequently, the regulatory authority has to estimate the level of exposure likely to be associated with the products' intended use in order to complete the risk assessment.

Although several studies have reported measurements of pesticide spray-operator exposure, they have largely been confined to determining the amount of chemical deposited on the external clothing and dispersed into the breathing zone. A further limitation of these studies is that they are conducted under conditions typical of the area considered and not necessarily relevant for other areas. In addition, the results of individual studies are only valid for the particular circumstances under which they were conducted and may not be representative of pesticide applications made on other occasions or at different locations. Consequently, the results of these studies are of limited use for estimating the exposure of spray operators to a new pesticide in different countries of Europe.

Variables to be used in the estimation of agricultural workers' exposure are dependent on the job being done, how it is done, the physical form of the pesticide, and the ambient conditions, rather than on its chemical nature. Main variables that may affect dermal and inhalation exposure have been identified in the following:

Type of activity:	Mixing/loading Application

	Flagging (for aerial application)
Type of application device:	Tractor-mounted
	Hand-held
Formulation:	Liquid
	Solid
	Gas
Condition of application:	Indoor
	Outdoor
Type of crop:	High
	Field
Temperature	
Humidity	
Wind	
Protection factors	Protective equipment
	Training/education

Moreover, the presence of co-formulates in the products is another factor that may affect exposure as solvents may act as vehicle for the absorption of the active ingredients. Finally, the formulates are often characterised by the presence of more than one active ingredient, and consequently, this fact introduces further complexity in the exposure assessment. For these reasons there is not an international agreement on a simple general algorithm to describe agricultural workers' exposure.

EUPHIDS' Agricultural Workers module is based on the use of Generic Databases. Generic databases are collections of exposure data produced by different field studies of exposure, performed under different conditions of use, with respect to the type of agricultural activity (mixing, loading, spraying), the type of formulation, and the type and mode of application. These exposure data sets allow the prediction of surrogate exposure levels for typical scenarios of exposure. The data-bases are descriptive in that they are based on data sets with which it is possible, using a suitable statistics, to estimate an exposure coefficient as a first step in risk assessment for registration. The underlying exposure data are not geographically homogeneous, since in each country exposure is assessed with the use of local equipment.

The external dose (ED) available for absorption is expressed as the amount (mg) of active ingredient that reaches the skin or is inhaled, per kg of active ingredient handled or applied (mg/person/kg a.i.).

The overall external exposure per work-shift, day or lifetime can be calculated by multiplying the ED for the amount applied/handled in the considered period of time, which, in turn, can be calculated from the kg a.i/ha recommended, the area of the treated fields, and the intended frequency of use.

For each route of absorption, the absorbed dose can be estimated by introducing a correction factor (k_{abs}) related to the variables influencing absorption. Among these, the chemical properties of the pesticide play a major role.

A European generic database is currently being created by a group of experts, which should review and pool all the available generic data that are representative of the European conditions and practices of use. The database will then be used to support a harmonised model, which will combine the best features of the existing models. Different subsets of the database will be used to support the differences in climate and working practices in different Member States. EUPHIDS is an open system, therefore, when a European database is available, it will be possible to include it in the system for a better harmonised evaluation.

It is important to recognise that the estimation using the generic database is usually an over-estimation of the actual operator exposure. The estimated exposure is compared with an Acceptable Operator Exposure Level (AOEL). The AOEL is derived from the toxicological data in a similar way to ADI using an appropriate margin of safety. For the purposes of protecting operators the AOEL will usually be based on No Observed Effect Level determined from the toxicological assessment. If an acceptable margin of safety to operators can be demonstrated, by comparing the estimated operator exposure level with the AOEL, then the crop protection product can be approved without further investigation. On the contrary, if this first estimate shows a non-acceptable margin of safety, actual data on specific model parameters should be used and actual field operator exposure studies should be conducted to determine the operator exposure and safety assessment more precisely.

4.1.3.2. Methodology

Several generic databases are in use in different countries. So far three principal models have been identified for the evaluation of agricultural workers exposure: the German model (BBA, 1988), the UK model (JMP, 1986) and the Dutch model (Van Hemmen, 1992). In EUPHIDS the decision maker may select between one of the models or, alternatively, he may let the three models run and consider the most conservative evaluation. At present only the German model has been implemented. It has been preferred to other models because the estimates are based on mean (geometric) values and not on the 75th percentile or the 90th percentile as in the UK and Dutch model respectively. A further improvement of the system could be the implementation of the other two models and, when available, of the European model.

Pesticide Handlers Exposure Database (PHED), a north American software tool designed to predict pesticide exposures, has been also considered during the implementation of EUPHIDS. This database is based on exposure data collected in a setting with agricultural characteristics rather different from those present in Europe: areas treated with pesticides in America are much larger than in Europe and planes are the major vehicle used to spread pesticides. For these reasons the use of PHED in EUPHIDS has not been considered to be appropriate.

4.1.3.3. German model

As already stated the German Model (BBA, 1988) has been selected as the first model to be implemented in EUPHIDS for the assessment of exposure of the Agricultural

Workers. The model considers scenarios of pesticide use. Exposure during application and exposure during mixing-loading are separately considered.

The external dose (expressed as the amount of active ingredient that reaches the skin or is inhaled per kg of active ingredient handled or applied) available for absorption is estimated for six different scenarios of exposure according to the intended or actual use of the compound:

1. Mixing/loading - hand-held exposure
2. Mixing/loading - vehicle exposure
3. Applicator - handled - upward exposure
4. Applicator - handled - downward exposure
5. Applicator - vehicle - upward exposure
6. Applicator - vehicle - downward exposure

Three routes of exposure are considered but the oral exposure has experimentally been accounted for by inhalation exposure. Estimated dermal and inhalation exposure for a defined working step depend primarily on the amount of active ingredient (a.i.) being handled. They are the product of the following values:

- the experimentally determined specific coefficient of exposure, k_{exp}, (obtained from the generic database) i.e. exposures related to handling 1 kg a.i., expressed as mg/person kg a.i.;
- the use rate of the a.i.;
- the area treated per day.

The module provides exposure evaluation for each commercial product containing the active ingredient under evaluation.

In order to enable the exposure evaluation, three different tables have been constructed. Table 4.4 collects the information on active ingredients and formulates, such as physical status, type of application, amount applied, etc.

Table 4.4. Pesticide table.

Pesticide	Name of the active ingredient
Formulate	name of the product
Status	physical status of the product (liquid, solid......)
Concentration of a.i.	g/l (or g/kg) of a.i. in the formulate
Rate of application	l/ha (or kg/ha) of applied formulate
Type of application	direction of application: upwards (u), downwards (d) or both (b)

Table 4.5 concerns the estimated exposure coefficients (k_{exp}, mg/kg a.i.) necessary for the evaluation of exposure in the different scenarios. As far as applicators' exposure is concerned, inhalation exposure is characterised by one k_{exp} ($k_{exp}(i)$) value, while dermal exposure presents three different k_{exp}, ($k_{exp}(d)$) to differentiate exposure for hand, body and head. Mixing/loading exposure is instead characterised by one value of k_{exp} either for inhalation or for dermal exposure.

In EUPHIDS, dermal exposure for applicators has been considered as the sum of the three different contributions of head, body, and hand. The k_{exp} values are strictly related to the physical characteristics of the formulate, and to the type of application (tractor mounted or hand held equipment).

Table 4.5. Estimated exposure coefficients.

Status	Type of activity	Type of application	$k_{exp}(i)$	$k_{exp}(d)$	$k_{exp}(d)$ (head)	$k_{exp}(d)$ (hands)	$k_{exp}(d)$ (body)
WG[1]	Mix/loading	Tractor mounted	0.008	0.02	-	-	-
WG[1]	Mix/loading	Hand-held	2	21	-	-	-
WP[2]	Mix/loading	Tractor mounted	0.07	6	-	-	-
WP[2]	Mix/loading	Hand-held	0.8	50[3]	-	-	-
Liquid	Mix/loading	Tractor mounted	0.0006	2.4	-	-	-
Liquid	Mix/loading	Hand-held	0.05	205	-	-	-
All	Applicator	Down - Hand-held	0.0011	-	0.062	0.38	1.6
All	Applicator	Up - Hand-held	0.27	-	4.8	11	25
All	Applicator	Down - Tractor mounted	0.0011	-	0.062	0.38	1.6
All	Applicator	Up - Tractor mounted	0.018	-	1.2	0.66	9.6

1) Wettable Granule
2) Wettable Powder
3) estimated provisional value

Table 4.6 identifies size scenarios of pesticide application, that is the areas that can be typically treated in one day under different application conditions.

Table 4.6. Area treated per day.

Description of application	Area treated (ha/day)
Upward - tractor mounted equipment	8
Upward - hand-held equipment	1
Downward - tractor mounted equipment	20

The handled amount (HA, mg/d) of active ingredient for applicators is therefore derived by the equation:

$$HA = (\text{Concentration a.i., g/kg}) \times (\text{Rate of application, kg/ha}) \times (\text{area, ha/d}) \times 10^3 \quad (4.4)$$

The mixing/loading exposure needs information on the amount of active ingredient handled that cannot be derived by other data. A default value of 1 kg/day of active ingredient has been used. Once obtained the HA of active ingredient per day, exposure can be evaluated by means of the estimated exposure values, k_{exp}, as follows:

$$\text{Dermal exposure (mg/day)} = k_{exp}(d) \times HA \quad (4.5)$$

Inhalation exposure (mg/day) = $k_{exp}(i) \times HA$ (4.6)

Once external exposure has been evaluated, a coefficient of absorption (k_{abs}, percentage) is introduced in order to estimate the absorbed dose through each individual route. If no specific data are experimentally available, for the commercial product under evaluation 100% absorption for the inhalation route is assumed as a default value, which represents a conservative approach. For dermal absorption, a 50% default value is assumed as default. When information on actual absorption is provided by specific studies, the user is allowed to enter the appropriate coefficient of absorption. The absorbed dose (inhalation or dermal) is then obtained as follows:

Dermal absorbed dose (mg/day) = $k_{abs}\,(d) \times k_{exp}\,(d) \times HA$ (4.7)

Dermal absorbed dose (mg/day) = $k_{abs}(d) \times k_{exp}(d) \times HA$ (4.8)

Inhalation exposure (mg/day) = $k_{abs}(i) \times k_{exp}(i) \times HA$ (4.9)

4.2. Assessment of the Health Risk

4.2.1. Introduction

As already mentioned, risk assessment in toxicology is based on hazard (toxicity) and dose-response evaluation combined with exposure assessment.

4.2.1.1. Toxicity assessment

The main goal of toxicity testing is the identification and proper description of the adverse effects caused by the pesticide in the different living organisms. Knowledge concerning the dose-response relationships for such effects is essential. Moreover, information on the mechanism of action should be obtained as this may allow more confidence in the extrapolation of the toxic effects among different species. Among regulatory bodies, a reasonable agreement exists concerning the basic methods and procedures of toxicity testing. In the European directive 91/414, the annexes II and III are expression of this agreement.

The widespread use of pesticides gives ample possibilities for such substances to come in contact with man either incidentally or intentionally, acutely or chronically, depending on their use, their persistence, and their migrating properties. The assessment of risk is then primarily based on three types of toxicity studies in animals:

- acute studies (which include LD_{50} determination) coupled with a description of the adverse effects;
- subchronic studies by different routes of administration;
- chronic studies (generally by oral or inhalation route) which are multidose one- two-year studies on rodents, dogs, or other relevant mammalian species.

The evaluation of results of toxicity tests, including their extrapolation to humans, is the cornerstone of health risk assessment. The result of animal experiments should be weighed for their significance to humans, since any animal model can be considered unsatisfactory due to the existing species differences. In the extrapolation from laboratory animals to humans, the followings aspects have to be considered: interspecies variation; intraspecies variation; extrapolation from high to low dose and experimental limitations. Assuming that a biological threshold can be identified for non-carcinogenic effects, both the acute and chronic data are then used to establish thresholds for the adverse effects of the pesticide; in most cases, the tolerances or other regulatory positions are established using an appropriate safety factor to divide the lowest threshold. The established No Observed Adverse Effect Level (NOAEL, mg/kg b.w.) from animal experiments, is therefore divided by a safety factor to compensate for the uncertainty of extrapolation, thus predicting a safe level for humans. Assuming that interspecies and intraspecies variations would each not exceed one order of magnitude, a "worst case" approach yields a safety factor of 100. This concept, used for almost forty years, has been shown to be sufficiently safe. Recently, the validity of a safety factor of 100 has been questioned: it might be too high since no evidence exists that the sensitivity of inter and intra-species variability are related. Moreover, present day toxicity testing is considered more advanced and generally results in NOAELs that are lower than those found decades ago. For pesticides, however, a conservative approach seems to be realistic, as long as this procedure is not applied too rigidly.

4.2.1.2.Evaluation

Two parallel evaluations have been implemented in EUPHIDS: on one side the assessment of the acute risk experienced by the workers during the agricultural practices, and on the other side the evaluation of risk of long-term effects which may follow chronic exposure to low doses of a compound, both among agricultural workers and among the general population. These two evaluations differ not only because of the population groups involved, but also because of the different implications on prevention and management of risk.

4.2.2. Risk assessment of acute effects

4.2.2.1.Background

The toxicological end-points which are taken into consideration by EUPHIDS for the evaluation of the acute risk to human health are the results of the short-term toxicological studies required in Annex II and Annex III.

These studies include the evaluation of:

- acute systemic effects, following absorption of a compound during a short-term exposure;
- acute local (irritative) effects, following the contact of a compound with the skin or the eye;
- sensitisation, that is the induction of allergic reactions following repeated contacts with the compound.

For each product, the following acute toxicity data are considered in EUPHIDS:

Acute systemic effects:

- Acute oral toxicity: oral LD_{50} in rat

- Acute dermal toxicity: dermal LD_{50} in rabbit
- Acute inhalation toxicity: inhalation LC_{50} in rat

Irritation assessment
- Irritative effects: dermal irritation test in rabbit
  eye irritation test in rabbit

Sensitivity assessment
- Sensitisation: sensitisation test in Guinea Pig

Moreover, results from human studies on acute toxicity can be considered, when available: in this case, an Effect Level can be entered, corresponding to the Minimum Observed Lethal Dose.

4.2.2.2. Methodology

In EUPHIDS, the characterisation of the acute-effect risk, has been implemented according to the following evaluations:

Sensitisation risk
On the basis of the results of sensitisation test in Guinea Pig, each compound is classified as "sensitising", "not sensitising" or "doubtful". When a NOEL for sensitivity assessment is available, it will be implemented in EUPHIDS.

Risk for irritative effects on skin
The irritative risk to skin is calculated as the ratio between the predicted dermal exposure (as mg/day) and the NOEL from dermal irritation testing on rabbit (mg/cm^2) multiplied by the surface of exposed areas (cm^2) as shown in Equation 4.10 Surface areas for regions of the adult body are provided as default values. In the case of gaseous formulations, a yes/no evaluation is provided.

$$\text{irritative risk} = \frac{\text{dermal exposure (mg/day)}}{NOEL_{irr}(mg/cm^2) \times \text{exposed area}(cm^2)} \tag{4.10}$$

Classification of toxicity
As a first risk evaluation, each compound is classified as "highly toxic", "toxic", or "harmful", according to the classification adopted by the EEC. This classification is based on the type of formulation (solid, liquid, gas), and on the LD_{50} provided by acute oral, dermal and inhalation toxicity animal testing.
According to the EEC recommendations, the classification into one of the three risk groups, implicates the adoption of specific preventive actions (e.g. need of a license, labelling requirements, protective clothing, etc.).

Percentage Toxic Dose
For each potential route of exposure (oral, inhalation, dermal), a "Percentage Toxic Dose" is calculated as the ratio between the predicted exposure level (oral, inhalation or dermal) and the corresponding LD_{50}:

$$\text{\% Toxic Dose (oral)} = \frac{\text{oral exposure(mg/day)}}{\text{oral } LD_{50} \text{ (mg/kg)} \times 70 \text{ (kg)}} \times 100 \qquad (4.11)$$

$$\text{\% Toxic Dose (dermal)} = \frac{\text{dermal exposure (mg/day)}}{\text{dermal } LD_{50} \text{ (mg/kg)} \times 70 \text{ (kg)}} \times 100 \qquad (4.12)$$

$$\text{\% Toxic Dose (inhal.)} = \frac{\text{inhalation exposure (mg/day)}}{LC_{50}\text{(mg/l)} \times \text{lung ventil. rate(l/h)} \times \text{Time(h/d)}} \times 100 \qquad (4.13)$$

A "% Toxic Dose" for cumulative exposure through all potential routes can also be calculated as the sum of the "% Toxic Dose oral, dermal and inhalation": this assumes an additive effect.

It is evident that the calculation of a "% Toxic Dose" is not used here (as in a typical risk evaluation) to estimate a ratio to the "acceptable dose": a Lethal Dose should just be avoided and therefore prevented in any way. Still, an estimate of how much the predicted exposure is far from the Lethal Dose may help in evaluating the actual acute risk (or, as a complement to 100%, the actual margin of safety) under the intended conditions of use. For instance, decision makers might state that when predicted exposure levels are $\geq$1% of the LD_{50}, the risk is not acceptable, and additional preventive actions are required. At present, in EUPHIDS only the "% Toxic Dose module" has been implemented as it was considered the most relevant evaluation to be considered in risk assessment. A further improvement might be the development of the other module which can give a global characterisation of acute effect risks. In Figure 4.3 is shown the flow-chart of the "% Toxic Dose".

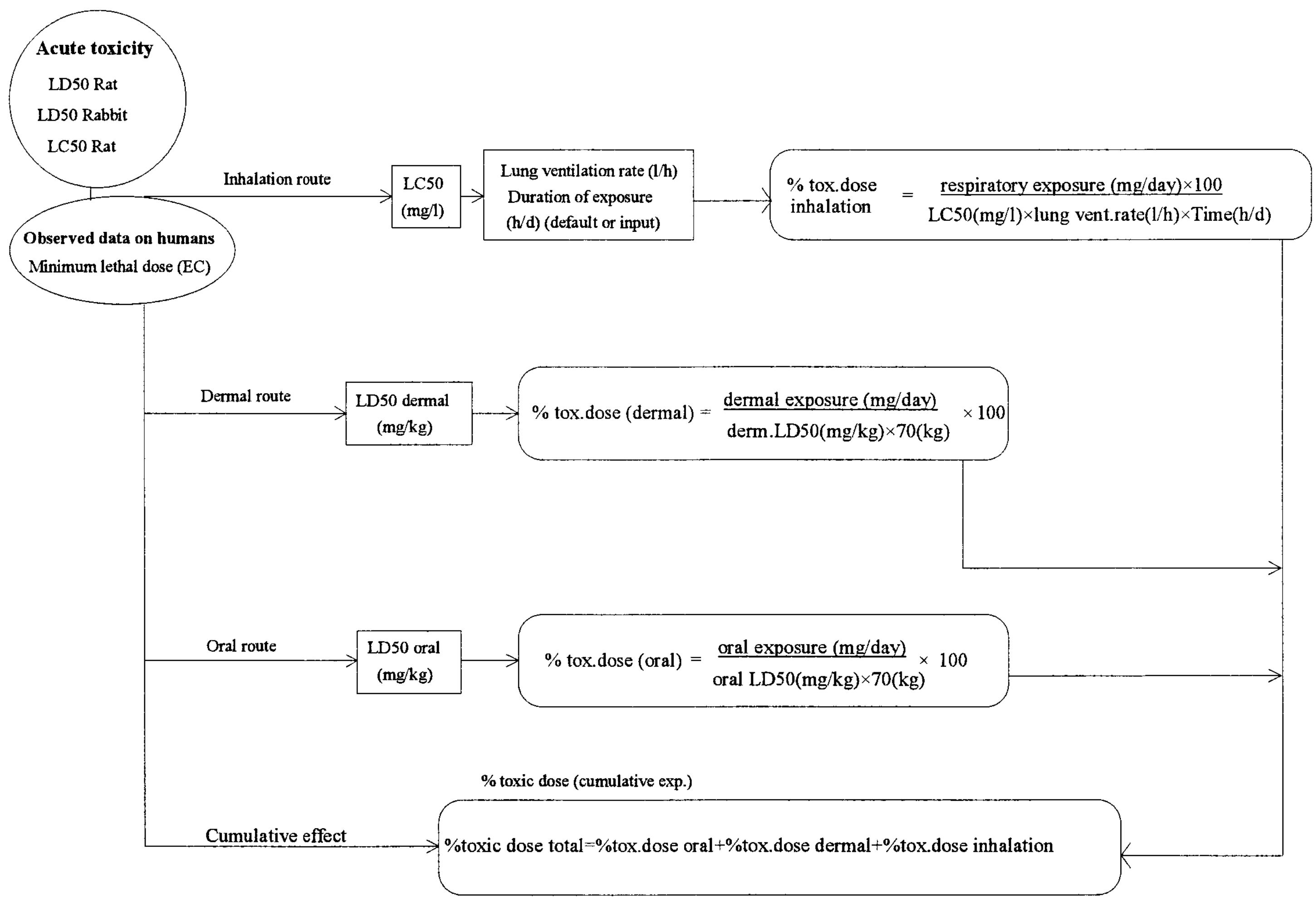


Figure 4.3. % Toxic Dose flow-chart .

4.2.3. Risk assessment of chronic effects

4.2.3.1. Background

Chronic exposure to pesticides can be expected by oral route for general population when residues of agricultural pesticides remain in food after application on crops or reach the food through environmental pathways. Agricultural workers and professional pesticide applicators are typically exposed by inhalation and dermal route to formulations and multiple compounds, either simultaneously or successively, often with an irregular frequency of application and under a great variety of conditions.
The basic question remains how to predict long-term effects on the basis of results of relatively short-term observations, and how to extrapolate data from laboratory animals to humans.

When long-term exposure of humans to pesticides is anticipated, acute and subchronic toxicity testing is not generally considered to be sufficient; in that case, chronic toxicity testing is necessary, as well as studies for such specific toxic responses as carcinogenicity, reproduction, toxicity, neurotoxicity, etc. The results of acute and subchronic tests should be thoroughly evaluated to determine which special studies need to be undertaken.

The toxicological end-points which are taken into consideration by EUPHIDS for the evaluation of the chronic risk to human health are the results of the toxicological animal studies required in Annex II. These studies include the evaluation of:
1. non-carcinogenic effects: for these effects it is possible to identify an exposure level (threshold) below which no effects are observed (NOEL);
2. carcinogenic effects: these are in general considered to be non-threshold effects, for which no exposure levels can be identified below which the effect does not occur. In some cases, mathematical modelling of the response function of the results of animal oncogenicity studies allows to calculate a "Unit Cancer Risk" (Q*), that is the excess risk (cancer frequency) associated with a lifetime exposure to a unitary dose of carcinogen.

4.2.3.2. Methodology

For each active ingredient, the following chronic toxicity data are considered in EUPHIDS:

- results of Subchronic testing (NOEL: when more values are available the lowest NOEL is considered);
- results of Chronic oral or inhalation studies (NOEL: as above);
- results of Developmental toxicity testing (NOEL: as above);
- results of Reproductive toxicity testing (NOEL: as above);
- results of in vivo Mutagenicity testing (NOEL: as above);
- results of Neurotoxicity testing (NOEL: as above);
- results of Oncogenicity studies (Q* or NOEL);
- the International Agency for Research on Cancer (IARC) classification of carcinogenicity (Group 1, 2a, 2b, 3, 4) is considered, when available, for re-registration of pesticides already in use;

- the Acceptable Daily Intake (ADI) established by the JMPR (when available);
- the Acceptable Operator Exposure Level (AOEL, when available).

As a further development these other classifications will be implemented:
- EEC classification of Carcinogenicity;
- classification of Mutagenicity;
- classification of Reproductive Effects
- classification of Oncogenicity.

Moreover, observed data in humans can be considered, when available. In EUPHIDS, the characterisation of the long-term effect risk, has been implemented according to the following evaluations:

4.2.3.3. Dietary Risk Evaluation (general population)

The evaluation of the potential risk to the general population is calculated as the ratio between the best possible prediction of dietary intake (TMDI/EMDI or EDI) and the Acceptable Daily Intake. When an ADI is not available, this is estimated from the lowest available NOEL; a Safety Factor (SF) is then applied to allow extrapolation from high to low doses and from species to species (a SF of 100 is used as a default value but it can be changed with any other desired value by the user).

$$\text{Potential risk} = \text{TMDI(EMDI or EDI)/ADI(or NOEL/SF)} \tag{4.14}$$

4.2.3.4. Exposure Risk Evaluation (agricultural workers)

The evaluation of the potential risk associated to operators' exposure under the proposed conditions of use is calculated as the ratio between the predicted absorbed daily dose and the Acceptable Operator Exposure Level (AOEL). When an AOEL is not available, this is estimated from the lowest available NOEL (mg/kg/day) multiplied by a default value for human body weight (70 kg); a Safety Factor is then applied to allow extrapolation from high to low doses and from species to species (a SF of 25 is the default value). Alternative NOEL values or Safety Factors can be chosen and entered by the user. This approach assumes an evaluation of risk of long-term effect resulting from a lifetime daily exposure. A correction can be applied to adjust for time, that is for the actual proportion of time during which exposure occurs. A Time Factor (TF) equal 1 is used as a default.

$$\text{Exposure Risk Evaluation} = \frac{\text{dose} \times \text{TF}}{\text{AOEL(NOEL/SF)} \times 70\text{(kg)}} \times 100 \tag{4.15}$$

4.2.3.5. Incremental Cancer Risk (general population and agricultural workers)

The evaluation of the excess cancer risk associated to long-term exposure is performed both for the general population and agricultural workers. For the general population, cancer risk is calculated as the product of Q* (i.e. the excess risk associated with a lifetime exposure to a unitary dose) by the best estimated daily intake (TMDI, EMDI, EDI) divided by a 70 kg default body weight.

For agricultural workers, cancer risk is calculated as the product of Q* by the predicted daily absorbed dose (divided by a 70 kg default body weight). A correction is applied to adjust for time, that is for the actual proportion of time during which exposure occurs (a TF of 1 is used as a default).

$$\text{Cancer risk(General Population)} = \text{TMDI(EMDI or EDI)} \times Q^*/70\text{(kg)} \qquad (4.16)$$

$$\text{Cancer risk(Agricultural Workers)} = \text{dose} \times Q^* \times \text{TF}/70\text{(kg)} \qquad (4.17)$$

In Figure 4.4 the flow-chart describing the above methodology is represented.

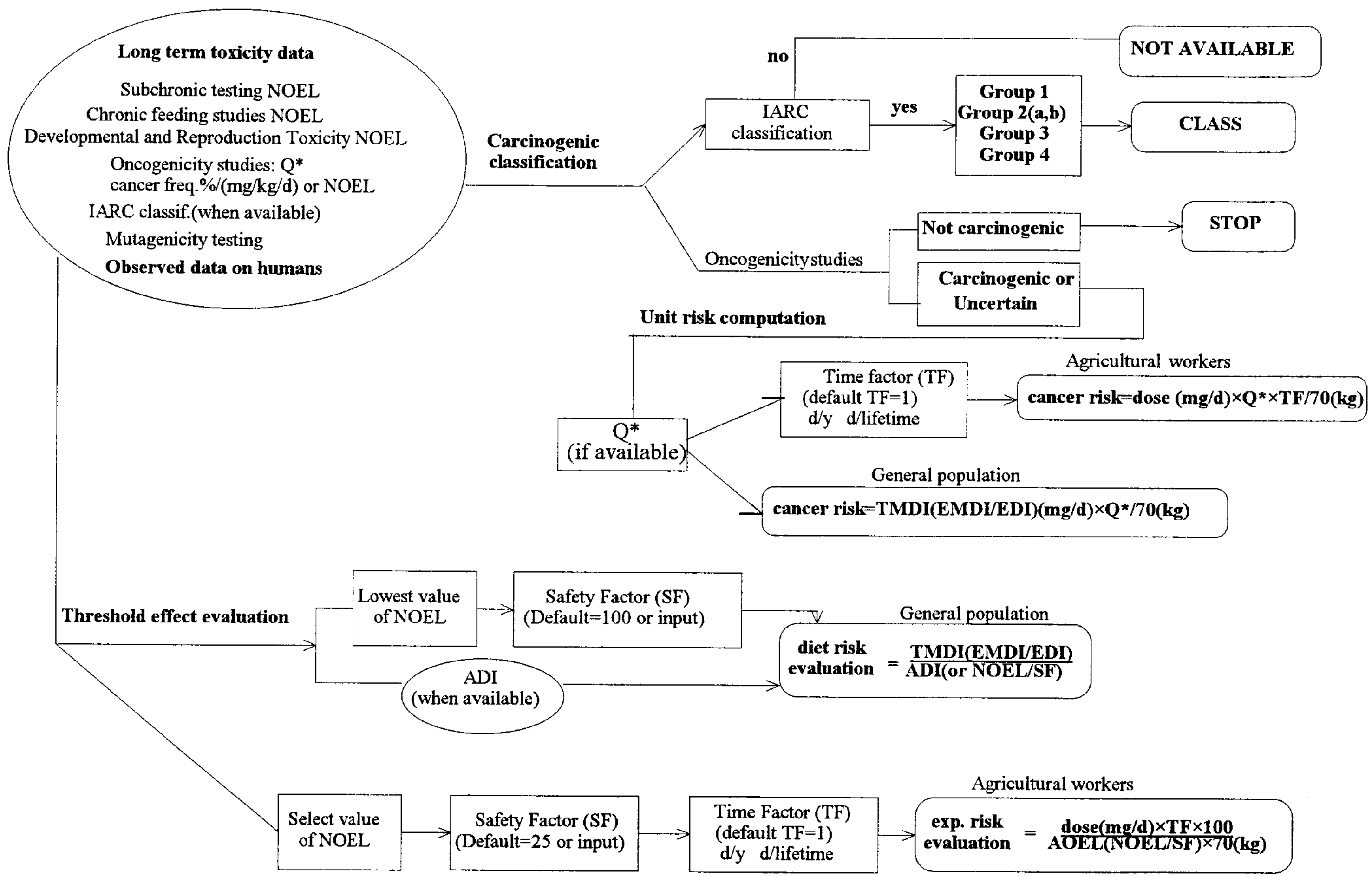


Figure 4.4 Long-term effects flow-chart

5. From spatial data to spatial information

5.1. *Introduction*

One of the key features of EUPHIDS is the spatial modelling of risk assessment. The objective of this chapter is to address the main issues related to this approach. In the whole process from spatial data to spatial information GIS is a crucial instrument for storing and processing spatial data, as well as the development of the spatial data model. For a more extensive overview on GIS perspectives, functionality and applications the reader is referred to Maguire *et al.* (1991).

In the spatial analysis of risk two elements are relevant: (I) the spatial scale of environmental and human health processes and (II) the regional differentiation of parameters underlying these processes. Both result in a spatial distribution of environmental and human risk. In order to know the spatial scale of the processes (I) the location of the field of pesticide application, the spatial scale of the exposure routes and the location of the receptors are relevant (cf. Chapter 3). With respect to the spatial scale of the processes two types of distances can be identified;

1. the location of the field of application corresponds to the location of the receptor (e.g., effects on the soil organisms of the field of application);
2. the location of the field is different from the location of the receptor (all other receptor groups).

EUPHIDS considers local and regional distances. EUPHIDS takes into account the interception, spray-drift, run-off and leaching processes resulting in effects on soil organisms in the agricultural field, effects on aquatic and terrestrial ecosystems adjacent to the field and effects on groundwater. The determination of the spatial scale of processes leading to human health effects is based on uniform diet regions.

The spatial processes taken into account in EUPHIDS are to various extents determined by variables that show spatial variability, such as soil, climatological circumstances and human food intake. Spatial models can be divided into those taking into account spatial interactions ('real' spatial models) and those models fed by spatially distributed parameters (static spatial models). In EUPHIDS all processes are modelled in a static manner. The run-off process, for instance, could have been modelled with spatial interactions, but such an approach appeared to be too data intensive and the state-of-the-art of data availability made their use problematic and of little practical relevance. EUPHIDS thus regionalises risk through the incorporation of spatial data in non-spatial risk assessment models. Space in EUPHIDS is represented as gridcells (or rasters). Within these gridcells values (of input data and thus outcomes) are considered homogeneous.

5.2. *The design of the spatial data model*

The creation of a data model is an integration of different raw data sources into one uniform, database in which all data layers are stored to meet the requirements of the process models and to perform the spatial analysis. In the design of the spatial data model the procedure depicted in Figure 5.1 is followed. The spatial data requirements are characterised by the data theme (or attribute, like, soil and slope), the resolution of the theme (indication of soil classes or subclasses) and the resolution of the areal unit (related to the spatial representation of the theme). These requirements are mainly determined by (I) model characteristics (scale of the model, type of model and the behaviour of parameters on the modelling outcomes), (II) data characteristics (spatial distribution of attributes, homogeneity versus heterogeneity) and (III) decision support requirements. After having identified the spatial data requirements data availability needs to be considered (IV). This whole process is often iterative. For instance, due to missing spatial data (identified in phase I and II), the data requirements need to be adjusted. The extent to which these requirements can be adjusted is dependent on the model and spatial data characteristics.

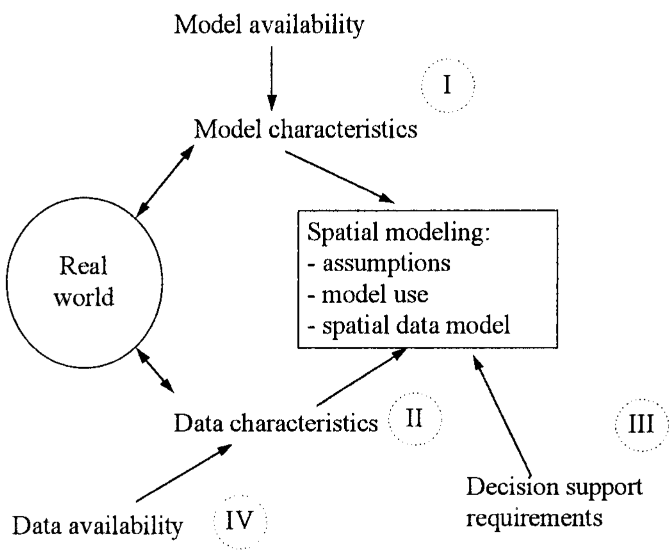


Figure 5.1. The design process of the spatial data model.

5.2.1. Model characteristics (I)

Chapter 3 and 4 addressed the processes and models implemented in EUPHIDS. The processes for which spatial parameters have been identified are run-off, leaching, top soil contamination, and the human intake. The model selected determines the spatial data themes. In the leaching models, for instance, spatial variables like soil and climate are involved. The modelling also put constraints on the resolution of these themes and the resolution of the areal unit. With respect to the latter it can be said that static spatial models in general offer more freedom in the selection of the resolution of the areal unit than 'real' spatial models. Other more spatial processes like run-off and drift were distance is involved are more complex and the freedom to select the scale of modelling is limited.

This degree of freedom in selecting areal units is often constrained. In the first place because of the scale of the model. Models can be scale dependent due to the processes incorporated; detailed models simulating large-scale processes versus more global models focusing more on the small-scale processes. A second constraint can be the behaviour of parameters on the outcomes. Parameters can be distinguished which are place dependent only and which have a direct influence on the outcomes of simulations. To this category belong soil properties like pH, percentage organic matter and slope. For these parameters more detail is allowed. On the other hand parameters can be place and time dependent and have a complex indirect influence on outcomes of simulations, like climatological circumstances. For these variables larger areal units need to be constructed (scenario's).

5.2.2. Spatial data characteristics (II)

The appearance of a variable in the real-world is relevant in the selection of an appropriate data model resolution. This appearance is related to the heterogeneity or homogeneity of a variable. From a spatial data perspective a data model should optimally represent the real-world appearance. Like process models also spatial data is characterised by a scale dependence. Climatological data, for instance, often does not show spatial variation at the local scale, in contrast to national and continental scales. To assess the most optimal representation often expert judgement is required. To be able to use expert judgement, existing data layers should be well documented with respect to items like, scale and composition in order to know their usability for the modelling purpose.

5.2.3. DSS requirements (III)

Already in the design phase of the spatial data model DSS requirements might play a role. Both the theme and the resolution of the theme determine to what extent decision questions can be dealt with. If, for instance, data is based on averaged values, a 'worst case' approach in decision making will be excluded. Thus, also the decision question determines the input data requirements. It should also be noted that existing data layers often already are aggregations from original data.

With respect to the spatial resolution of data other factors play a role. EUPHIDS enables the user to analyse impacts of a decision (in this case selection of pesticide) interactively. Interaction requires a good system performance. The more detailed the spatial data layers the more time the system will need to perform these calculations.

5.2.4. Spatial data availability (IV)

It can be difficult to obtain the data themes as well as the appropriate level of resolution of themes (in particular for larger areas, like Europe). When data is missing either other modelling approaches can be chosen (this reflects the interactive process of spatial data modelling) or a more rough approach can be chosen, by making assumptions for larger areas (also referred to as scenarios). The spatial data layers presently implemented in EUPHIDS reflect a hierarchical data model: more detailed data in regions, more global data at smaller scales (see section 5.5).

5.3. Spatial data requirements of EUPHIDS

Table 5.1 shows the spatial data themes required to assess the PEC groundwater, PEC aquatic ecosystems (long term and short term) and the EDI for the general population.

The spatial parametrisation to calculate the PEC soil is a future development of EUPHIDS. In addition to the data layers presented in Table 5.1, some optional data layers can be linked to EUPHIDS: landuse maps (for pre-selecting areas of potential pesticide use) and maps containing administrative regions (for aggregating outcomes and presentation purposes).

As described in Section 5.1 the run-off and human intake processes in EUPHIDS are modelled by spatial parametrisation. The algorithms used are fed with the spatial data described in Table 5.1 (see also Chapters 3 and 4). An exception is the leaching process which is dealt with in two steps (cf. Chapter 3). First, the models (PESTRAS and PELMO) are run for a particular soil-climatological reference situation. The model outcomes are assumed to be applicable to larger areal units (scenario's in Table 5.1) having the same climatological, soil and landuse characteristics as the reference situations. Then, the model outcomes are further regionally differentiated within the model region (see Chapter 3). The main reasons for the use of scenario's are considerations discussed in section 5.2: the indirect influence of mainly climatological parameters on model outcomes (I; Figure 5.1) and the DSS requirements to enable fast calculations in EUPHIDS (III; Figure 5.1).

Table 5.1 Spatial data requirements EUPHIDS.

Exposure	**Process model**	**Spatial data (scenario's)**	**Spatial data**	**Required file format**
PEC surface water (long term and short term)	drift, run-off	-	- sand-stone - slope - max. rainfall of the month of application- organic matter content (%)	GRIDASCII
PEC groundwater	leaching (PESTRAS, PELMO)	- soil climate regions	- organic matter content (%)	GRIDASCC
EDI general population	human intake	-	- diet regions	UNGENERATE (and getpol)

EUPHIDS requires the grid data structure for calculations and display. This representation is selected as it enables easy and fast map computation and analysis. Scientific considerations (model and data characteristics) should in principle guide the selection of the number of model regions as well as the resolution of the gridcells of the spatial data shown in Table 5.1. The modelling assumptions made in EUPHIDS (Section 5.2) allow various resolutions of the areal unit, except the very field scale (smaller than 100 by 100 meters). This implies that the resolution of the gridcells is determined by the spatial variation in data. As seen above, availability of spatial data and DSS requirements can result in other choices for other (larger) gridcell resolutions. Section 5.5 further describes the spatial information in EUPHIDS.

Table 5.1 also describes the spatial data file format needed to import the data in EUPHIDS. Both GRIDASCII and UNGENERATE are Arc/Info commands (ESRI, Redlands, USA). Getpol is a C programme supplied with EUPHIDS to convert the UNGENERATE file.

5.4. *The organisation of spatial modelling in EUPHIDS*

In the development of EUPHIDS two phases can be distinguished (see also Chapter 2): (1) the development of the spatial data model and the development of spatial process, evaluation and presentation models, and (2) the integration of the different components in EUPHIDS. The objective of this section is to illustrate these two phases from a spatial data and spatial modelling perspective with the example of the calculation of PEC groundwater. The input data, operations and output have already been described in Chapter 3.

5.4.1. Development: modelling in GIS

Figure 5.2 depicts the steps (shaded objects in figure) in the spatial modelling of the leaching process: the storage of raw data (climatological information, soil type information and landuse information), the data integration and leaching calculations.

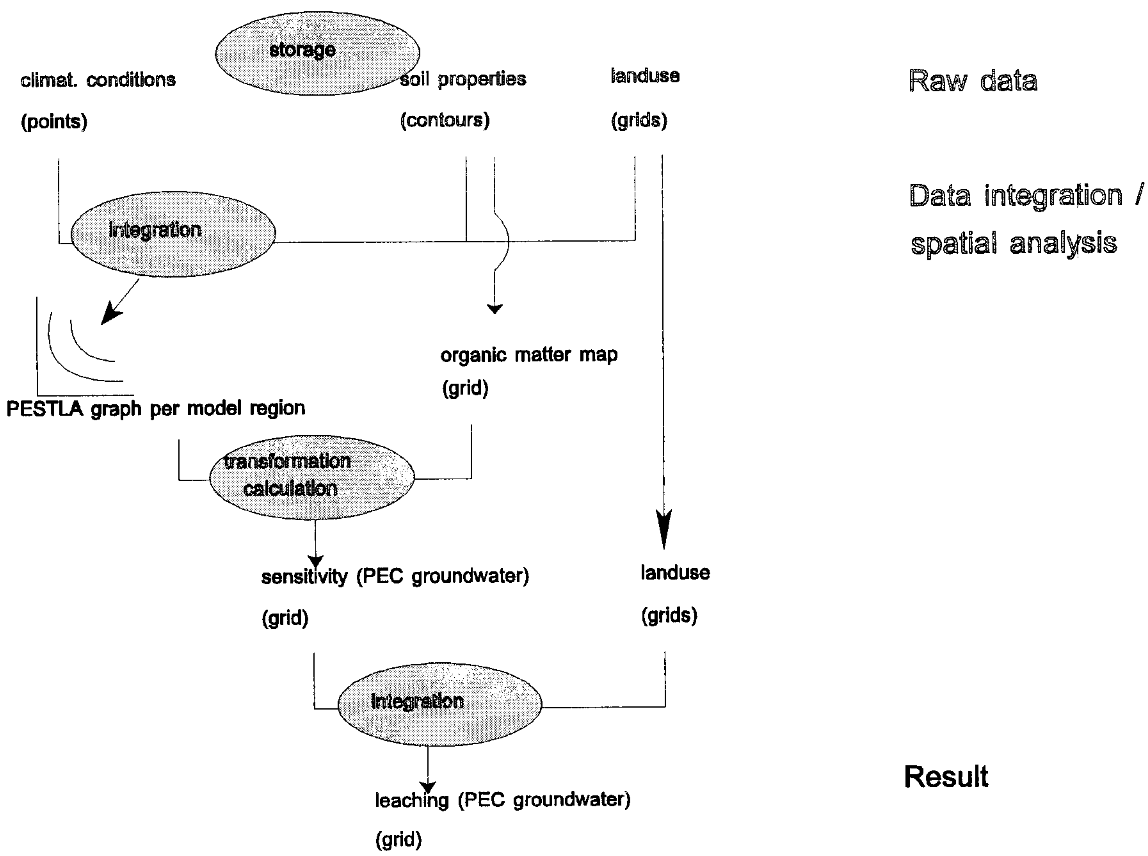


Figure 5.2. Spatial modelling of the leaching process (preparation phase).

The modelling process is time consuming and often demanding a large number of highly specialised operations, such as projections, interpolations, overlays. These operations need to be carried out with sophisticated GIS software. In the project the Arc/Info system is used for this purpose. The outcomes of the PESTRAS and PELMO models (the leaching graphs per scenario) are linked to Arc/Info and used for further regionalisation within scenario's and visualisation of the outcomes.

5.4.2. Transfer to the decision maker: modelling in EUPHIDS

The second phase involves the integration of the different components developed in the first phase into EUPHIDS. Figure 5.3 depicts in a schematic manner how calculation of the PEC groundwater is handled in EUPHIDS. Generated spatial data layers (the identified model regions and the percentage organic matter map) are the input from GIS. Only the results of the process models (the leaching graphs per model region) are implemented in EUPHIDS in order to increase the systems performance. The regionalisation of pesticide leaching within model regions takes place in EUPHIDS, taking into account the selections entered by the decision variables in the user-interface. This design of the system implies that users need GIS and the PESTRAS or PELMO model to generate the required information to make risk assessments for new areas.

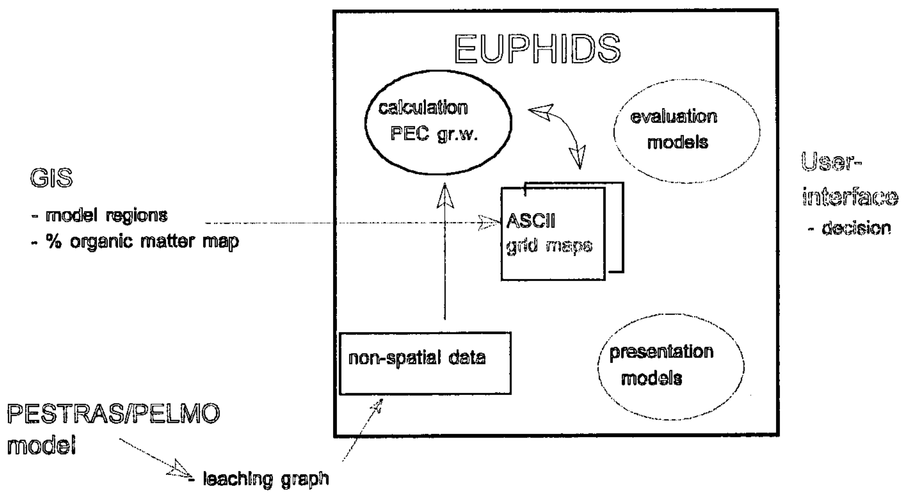


Figure 5.3. Spatial modelling of the leaching process (EUPHIDS).

5.5. *Data availability within the project*

EUPHIDS is designed in such a way that pesticide risk assessment and evaluation can be performed for any region. To test the methods and techniques developed in the project, spatial information for specific regions has been collected and stored. To test modelling results for multiple scales three spatial levels have been selected (Europe, national, regional). The national and regional areas are selected because of availability of knowledge (e.g., test results, monitoring information). The regions identified are: Europe, The Netherlands, Germany, Italy, Hupselse Beek (The Netherlands), Kreis Soest (Germany) and Parco Sud di Milano (Italy). Table 5.2 gives an overview of the spatial information collected. This information is included in EUPHIDS.

Based on the considerations described before (model and data characteristics, DSS requirements and data availability) the EUPHIDS spatial data model has been designed. This resulted in a hierarchical data model. Figure 5.4 depicts this hierarchical data model, as well as the areal unit resolutions of the gridcells of the first five spatial data layers of Table 5.2. For the regional and national spatial data layers this resolution has been selected based on expert judgement. The resolution of the European information is aggregated to gridcells of 10 * 10 kilometres so as to improve the performance of the system.

Table 5.2. Current spatial data layers in EUPHIDS.

Regions /Spatial information	Europe	The Netherlands	Germany	Italy	Hupselse Beek (The Neth.)	Kreis Soest (Germ.)	Parco Sud (Italy)
landuse	x	x	x	x	-	-	-
sand-stone	x	x	x	x	x	x	x
slope	x	x	x	x	x	x	x
maximum rainfall of month of application	x	x	x	x	x	x	x
organic matter content (%)	x	x	x	x	x	x	x
soil-climate regions (leaching)	x	x	x	x	-	-	-
diet regions	x	-	x	x	-	-	-
administrative regions	x	x	x	x	-	-	-

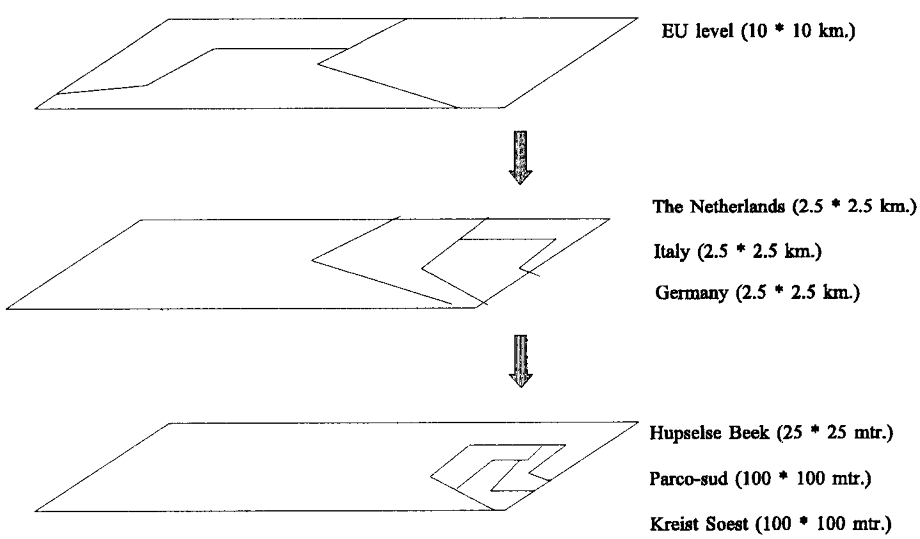


Figure 5.4. The multi-level structure spatial data model.

Further information on the source information of the data layers shown in Table 5.2 can be found in Appendix A4: "Meta information on spatial data". This includes the source of information, the method of compilation (estimations or measurements), the spatial object (point, line, areas or grids) and their attributes as well as an indication of the accuracy of the data. It also informs about the GIS operations performed to arrive at the EUPHIDS data layers.

6. A guided tour of EUPHIDS

6.1. Introduction

This chapter shows a typical sequence of operation in EUPHIDS. The main possibilities offered by the system are briefly illustrated and an overview of its main inputs and outputs are provided. The reader is referred to the previous chapters and to the technical manual for a detailed description of EUPHIDS.

EUPHIDS requires two types of inputs: system inputs and user inputs. System inputs refer to the information built into the system which is necessary to run the program. This includes geographical information for the areas studied (for instance, the soil, climate and slope maps for Europe, Germany, Italy, the Netherlands etc.), information on the pesticides analysed (for instance, the chemical, toxicological and ecotoxicological characteristics of Atrazine, Bentazone etc..) and the models to compute environmental and human exposure levels to the pesticides used. In general, the user does not need to change this information, apart from adding a new substance to the system or a new area for evaluation.

The user inputs are the parameters which need to be specified for the question at hand. These include, for example, the pesticide, the application dose, the choice of application type among those offered by EUPHIDS (spray, granules etc.), the exposure times for the species analysed and so on.

EUPHIDS is composed of five main modules: the initialisation module, the environmental module, the human health module, the evaluation module and the analyse output module. Before proceeding with these modules, the user needs to specify the area for which the analysis has to be made, the pesticide and dose applied. In this chapter, several areas, pesticides and application doses will be used to show the capabilities of EUPHIDS.

6.2. Initialisation

To initialise operations in EUPHIDS one must choose the relevant area, pesticide and dose used. These choices form the main settings for all subsequent operations. The area, pesticide name and dose are always displayed on the bottom left of the screen of EUPHIDS. The *initialisation* module serves to set the global parameters and types of effects for the computation of environmental and human health exposure for the pesticide and area under evaluation (Figure 6.1). The initialisation also sets the mathematical models used to compute the environmental and human exposure to the pesticide. Once the global settings are specified, EUPHIDS allows the computation of environmental concentrations and of human exposure levels. This is done in the *environment* and *human health* modules.

6.3. Calculation of environmental concentrations

The first operation in the *environment* module is selection of the parameters for computing environmental concentrations for long and short term exposure (Figure 6.2).

EUPHIDS offers the possibility of computing environmental concentrations for top soil, groundwater and surface water, under different application types, exposure times, physico-chemical and biological characteristics of the compound. After selecting the relevant and appropriate parameters for the prediction models, EUPHIDS computes the PEC (Predicted Environmental Concentrations) for short and long term. These results are presented in a series of maps. A typical result is shown in Figure 6.3, for groundwater. The maps shows four classes of Atrazine concentrations in groundwater. Similar results can be obtained for concentrations in surface water and top soil.

6.4. Calculation of human exposure

Human exposure to the pesticide occurs via ingestion of food or water containing pesticide residues (general population) or via direct exposure to the chemical compound (agricultural worker). EUPHIDS contains models for computing both exposure levels, which lead into two types of results. The general population module, on the basis of diet information, provides information of the daily intake of the compound (TMDI: theoretical maximum daily intake; EMDI: estimated maximum daily intake; EDI: estimated daily intake) and results in maps showing the spatial distribution of intakes on the basis of diet regions (Figure 6.4). The agricultural worker module provides estimates of the external and absorbed doses due to direct handling of the compound. The result is a series of tables which show the dermal and inhaled dose of the substance on the basis of the quantity handled and the type of application (Figure 6.5).

6.5. Evaluation module

6.5.1. Types of evaluation

The evaluation module aims to produce risk indices to support the assessment of acceptability of environmental and human health effects.. The evaluation scheme includes the guidelines of the Uniform Principles, which specify for each aspect under evaluation a risk threshold (a reference level). The evaluation is based on the risk ratios between the exposure and the risk threshold. For instance, the risk to groundwater is represented by the risk ratio (PEC groundwater)/(drinking water standard for groundwater): if the ratio exceeds one, then there is, by definition, the risk of unacceptable pollution levels in groundwater. This approach can be applied to different aspects (e.g. groundwater pollution, human health etc.); different targets (e.g. single species, ecosystems etc.) and can be considered for long and short term exposures.

Environmental evaluations are based on four types of analysis: the risks to single-species (for instance, the risks to fish in surface water); the risks to ecosystems (for instance, the risks to terrestrial ecosystems); the overall risks due to the combination of simultaneous risks in multiple environmental compartments (e.g. groundwater, top soil, surface water) and analysis of spatial trends in risks. The first two evaluations are based on risk ratios. The third, also called integrated risk analysis, is performed with value functions. The initial evaluation screen in EUPHIDS is shown in Figure 6.6. The input data for all the evaluations are the output maps of the *environment* module (the PEC maps for top soil, surface water and groundwater) and of the *human health* module (the TMDI, EMDI and EDI maps)(Figure 6.3, Figure 6.4, Figure 6.5).

6.5.2. Evaluation of environmental effects

The simplest evaluation is the computation of the risk ratios for individual organisms. For this purpose, EUPHIDS stores the ecotoxicological end-points, in the short and long term, for each pesticide. As shown in Figure 6.7, for fish, daphnia, algae and earthworms, EUPHIDS displays the available ecotoxicological end-points and suggests a corresponding (N)EL. The (N)EL or EL levels or safety factors (according to the UP) are used as thresholds by which to compute risk ratios. Figure 6.8 shows the risk ratios for groundwater according to the UP (threshold=0.1µg/l). The green area corresponds to risk ratios lower than one (no risk), while non-green areas show ratios higher than one (risk). Similar maps can be obtained for individual taxa (species) such as fish, algae and crustacean in surface water or earthworms in top soil, for both the short and long term.

The risk ratio approach can be applied to more aggregated evaluations, with the introduction of ecosystem risk thresholds. This requires the calculation of a (N)EL at the ecosystem level. Exceeding this (N)EL level indicates that surface water and top soil environmental compartments are exposed to risk. The risk threshold for ecosystems is based on the sensitivity levels of the organisms in the ecosystem and accommodates concepts such as protection of the weakest link in the chain. EUPHIDS offers three possibilities for computing the ecosystem risk threshold: the EPA method, the safety factors method (equivalent to the EPA, apart from the possibility of using user-defined safety factors) and the Sensitivity Distribution method. This evaluation results in risk maps for top soil and surface water long term (Figure 6.9). Similar maps can be obtained for short term risks.

The single-species (taxa) and the ecosystems threshold analysis offer two levels of risk evaluation. These two approaches are more useful for highlighting the existence of risk (yes-no decisions) rather than for measuring risk intensity. In contrast, integrated risk assessment does aim to measure the overall risk intensity to which multiple environmental compartments are simultaneously affected (for example, the overall environmental risk combining contamination of groundwater, surface water and top soil pesticide). This analysis is performed in EUPHIDS with value functions. For each compartment (groundwater, top soil and surface water), a value function translates PEC scores into a value score which ranges from 0 (unacceptable risk) to 1 (no risk) (cf. Chapter 3). This results in a value map for each environmental compartment. Multiple value maps are combined through a weighted combination, where the weight represents the relative importance attached to the individual risks. For instance, the long term environmental risk is a weighted combination of long terms risks to top soil organisms, surface water organisms and groundwater. Figure 6.10 shows examples of value functions for long term risks to top soil, groundwater and surface water. The bars at the right hand side of each function represent the weights attached to each single aspect. The weight attached to groundwater, for instance, reflects the importance of keeping groundwater clean against the importance of limiting effects on top-soil and surface water organisms. Value functions and weights are assessed on the basis of existing knowledge and expert judgement. EUPHIDS provides a database of value functions for each pesticide included in the system. The result of the aggregation is an overall risk map which shows, for each grid cell, the overall environmental risk (Figure 6.11). In this example, almost every portion of the area under evaluation (the Netherlands) is exposed to some risk due to the combination of risks in groundwater, top soil and surface water. Also, a rather significant part of the area is exposed to high risks, close to or exceeding the maximum risk threshold (red areas).

6.5.3. Evaluation of human health effects

The evaluation of human health effects is based on the classification of the effects of the substance (IARC classification), on calculation of the cancer risk (for carcinogenic substances) and of the risk ratios for the exposure levels. The EUPHIDS database provides this type of information for each pesticide. The risk ratios are computed by comparing the exposure levels (TMDI, EMDI or EDI) with the ADI level (Admissible Daily Intake) threshold.

For the general population this results in a map which shows the risk ratio per diet region (Figure 6.12). For agricultural workers, the outcome is presented in the form of a table, where the risk ratios are presented in different colours (Figure 6.13)

6.6. Analysis of output

EUPHIDS processes large amounts of information and produces many results. The *analyse output* module provides a collection of the main inputs and outputs of EUPHIDS, especially for the spatial information (Figure 6.14). EUPHIDS offers several options for displaying maps and addressing the spatial evaluation of information. Spatial evaluation deals with the distribution of risks and aims at capturing the relevant insights to the spatial patterns and regularities of risk distribution. EUPHIDS supports three types of spatial evaluation: filtering, uncertainty analysis and spatial aggregation.

Filtering highlights uniform areas which have limited variability in their risk levels by mapping with lower degrees of fragmentation. This can be used to isolate areas with similar information and help the interpretation of the map. Figure 6.15 shows the result of filtering for the groundwater risk map. Areas in green on the map indicate areas with similar risk levels.

The uncertainty option serves to test the robustness of risk ratios. Figure 6.16 shows the result of uncertainty analysis applied to the groundwater risk map. An uncertainty factor of 70% is assumed for the PEC levels. The resulting map shows the areas where the PEC remains below the threshold (0.1μg/l), where the PEC exceeds the threshold and where classification below or above the threshold is impossible due to uncertainty.

Spatial aggregation serves to provide risk indications at aggregated spatial units (for instance, municipalities, provinces, soil types etc.). Figure 6.17 shows the result of the spatial aggregation of risk ratios for groundwater at the municipality level. Within each municipality, EUPHIDS computes the average of the risk ratios and produces a map which shows the results within each municipality contour.

In addition to these analyses, statistical evaluations can be performed for each type of map. Statistical analysis can be used to count the number of grid cells in each class or to calculate the cumulative distribution of cells into classes (Figure 6.18).

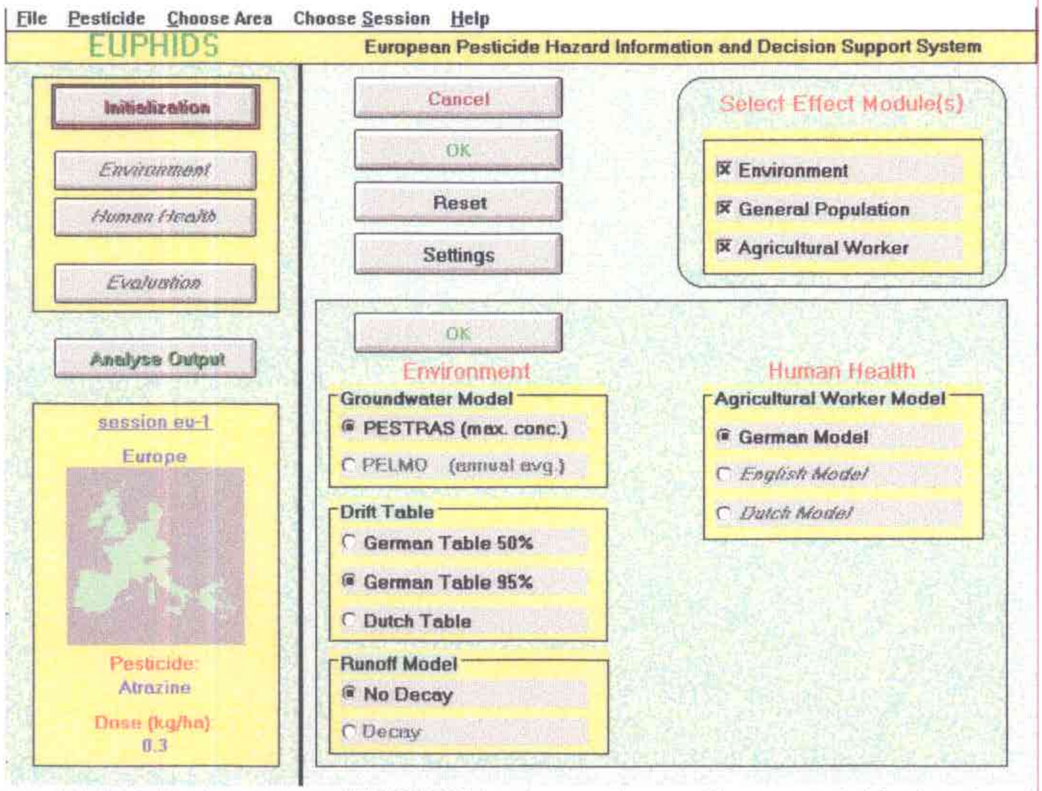


Figure 6.1. Initialisation screen of EUPHIDS (session: eu-1; area: Europe; pesticide: Atrazine; dose: 0.3 kg/ha).

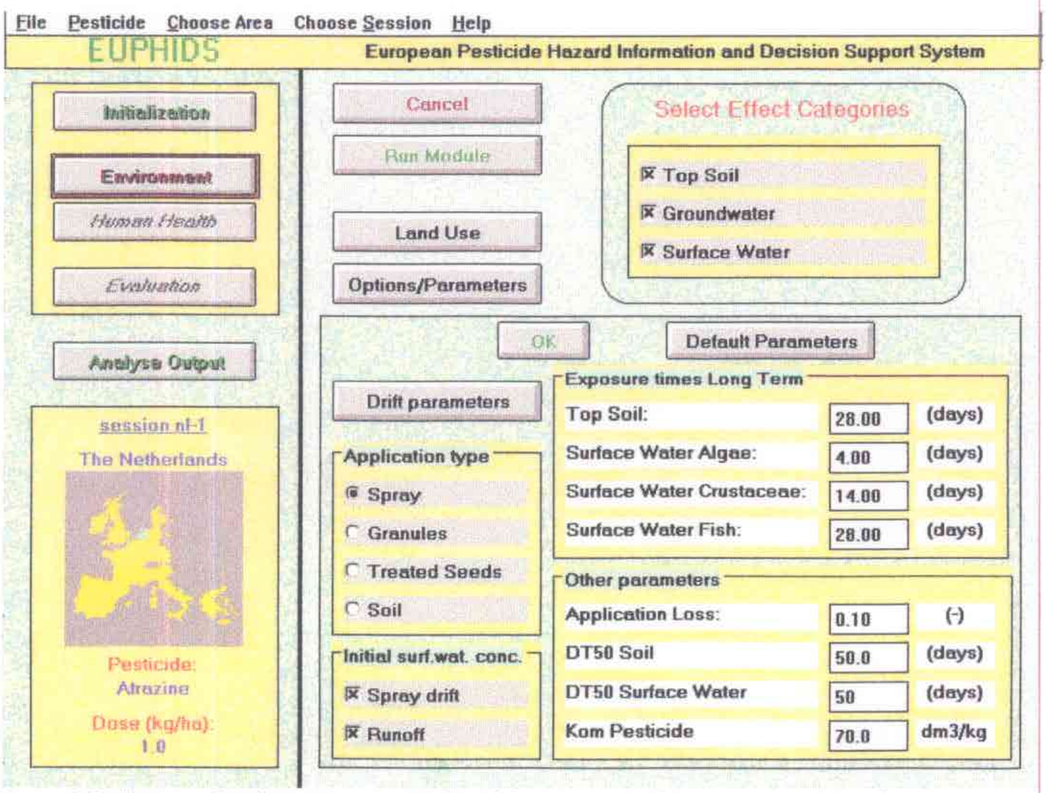


Figure 6.2. Settings for the environmental module (session: nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

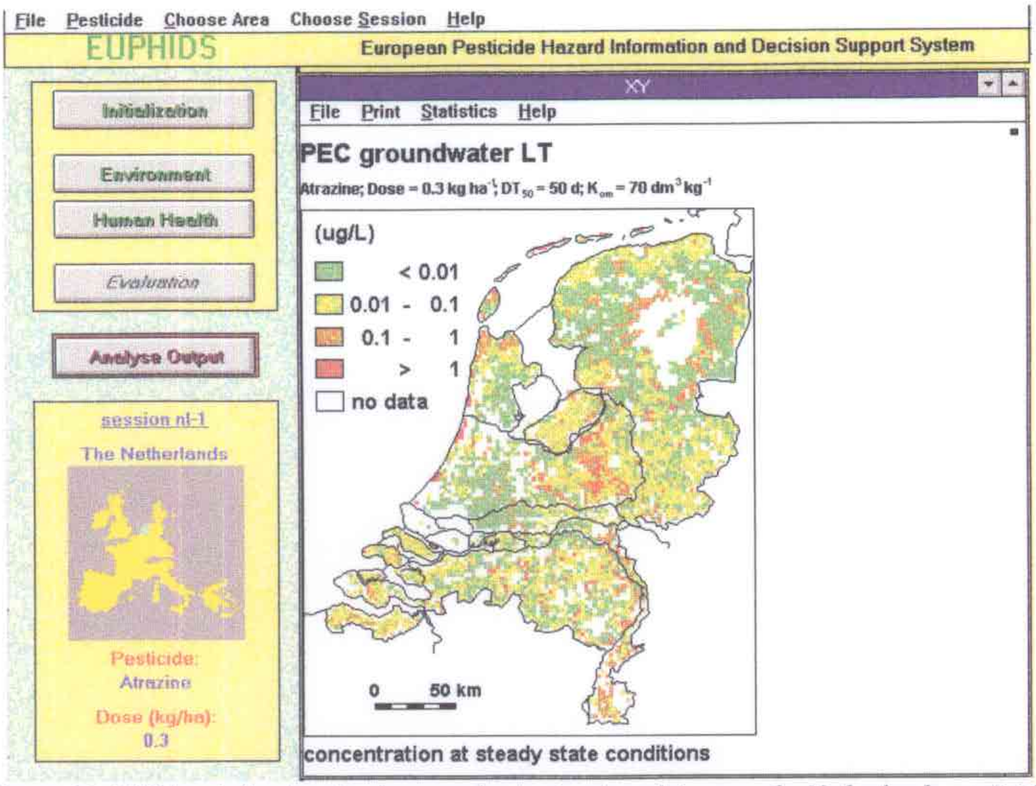


Figure 6.3. PEC levels for Atrazine in groundwater (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

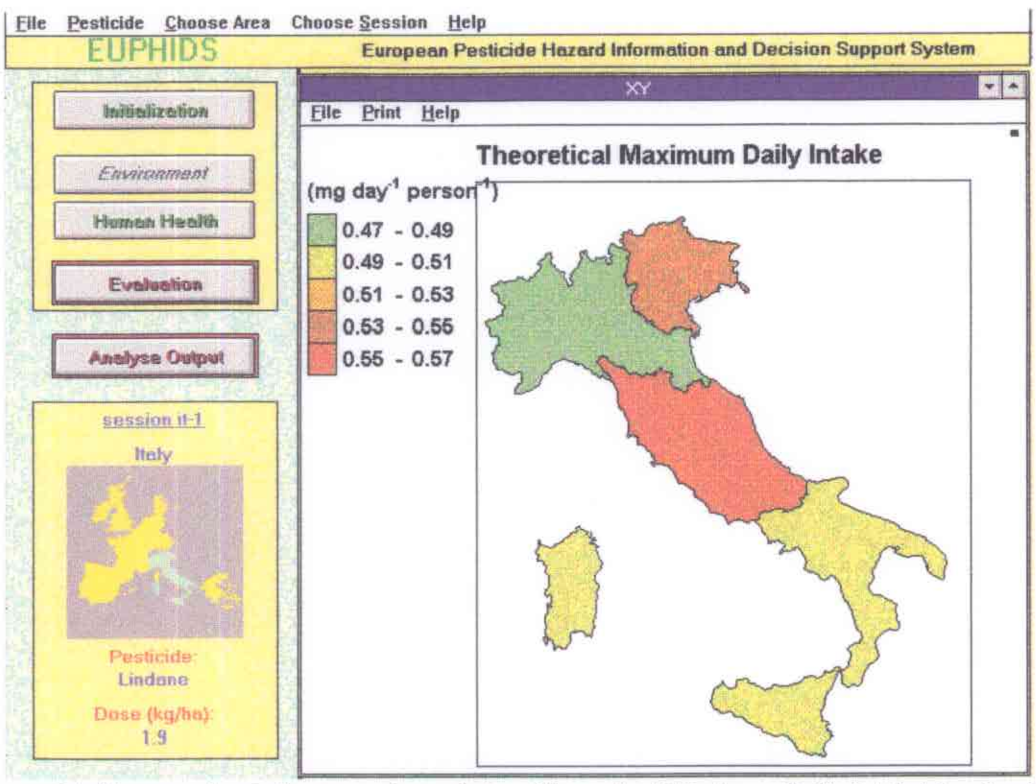


Figure 6.4. Exposure levels for general population (Theoretical Maximum Daily Intake) (session it-1; area: Italy; pesticide Lindane; dose: 1.9 kg/ha).

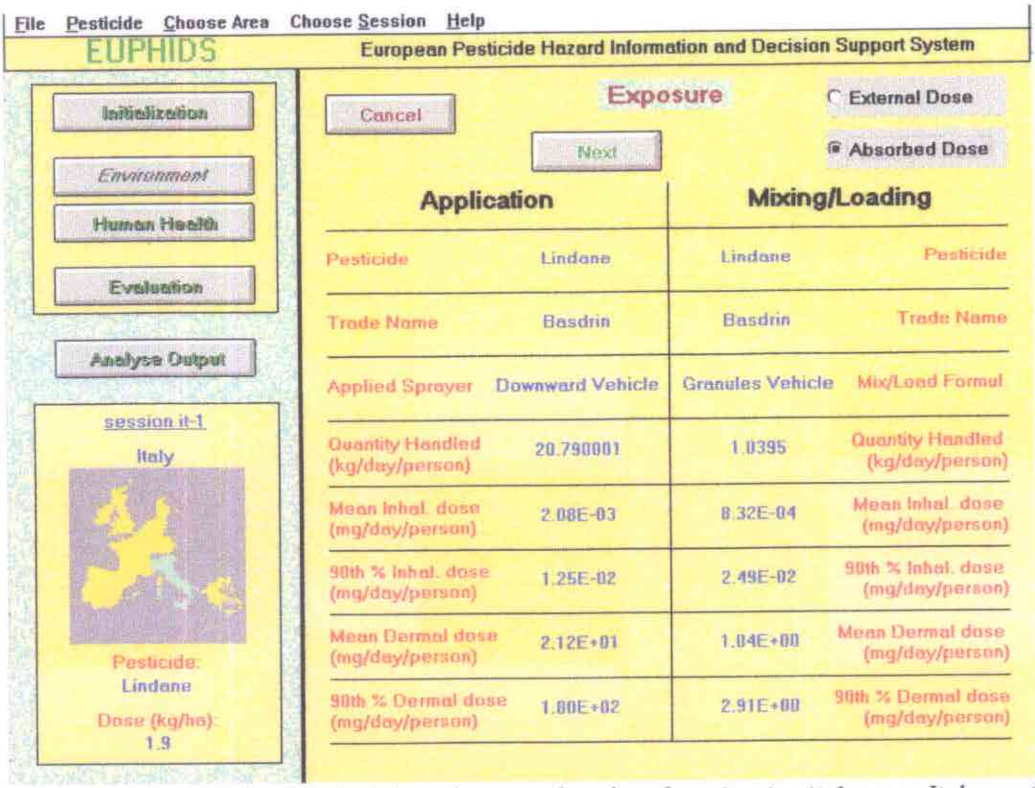


Figure 6.5. Exposure levels (absorbed dose) for agricultural workers (session it-1; area: Italy; pesticide Lindane; dose: 1.9 kg/ha).

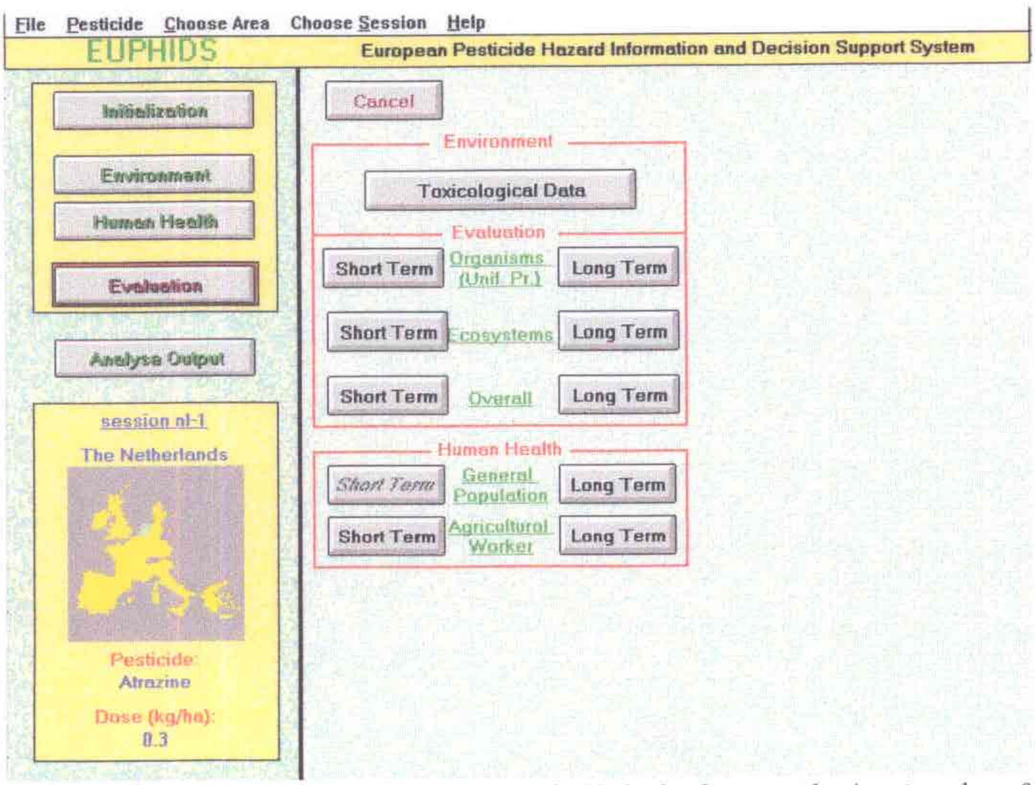


Figure 6.6. Evaluation screen (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

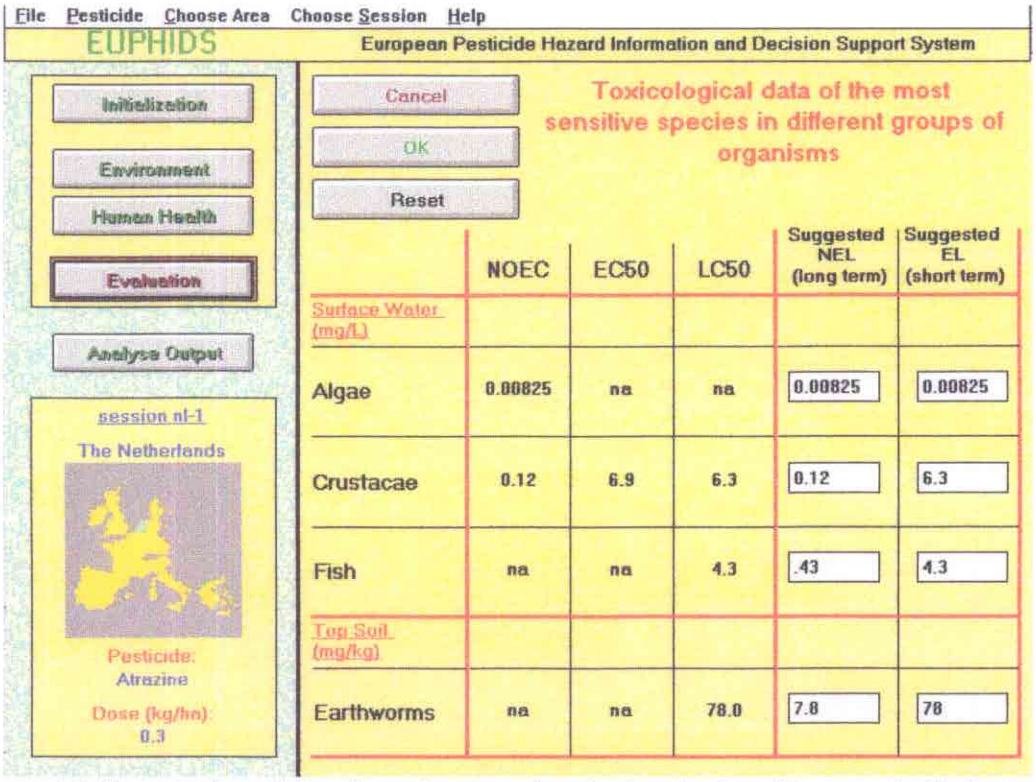


Figure 6.7. Ecotoxicological data for environmental evaluation (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

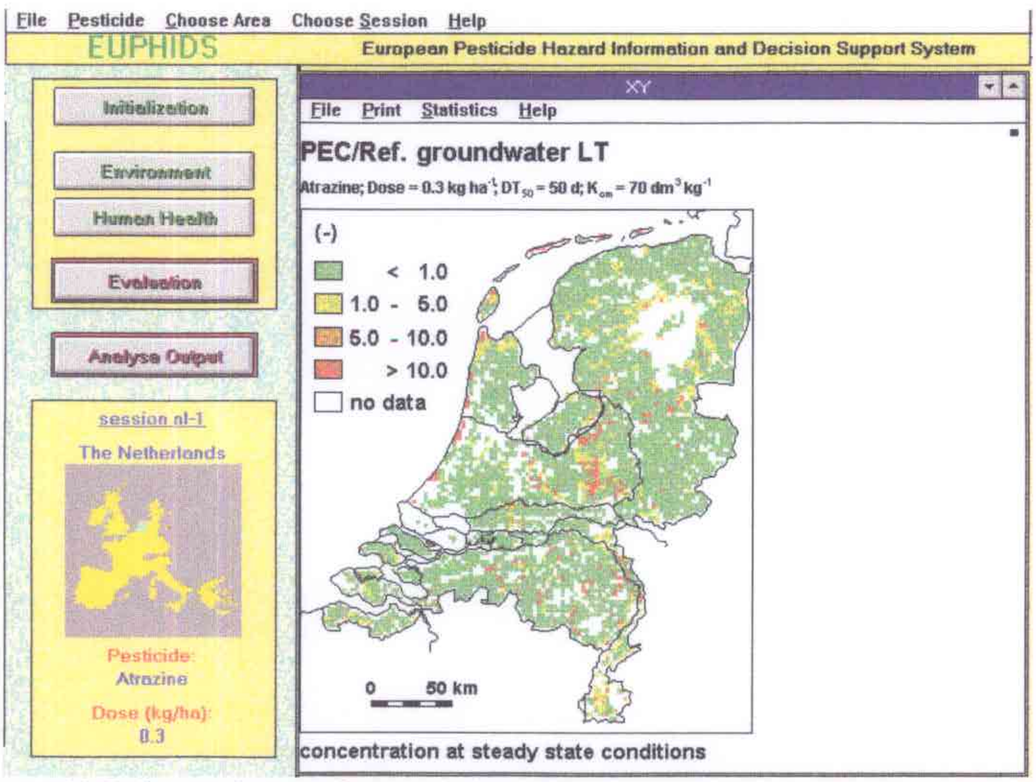


Figure 6.8. Risk ratios for groundwater with threshold evaluation (threshold=0.1 µg/l) (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

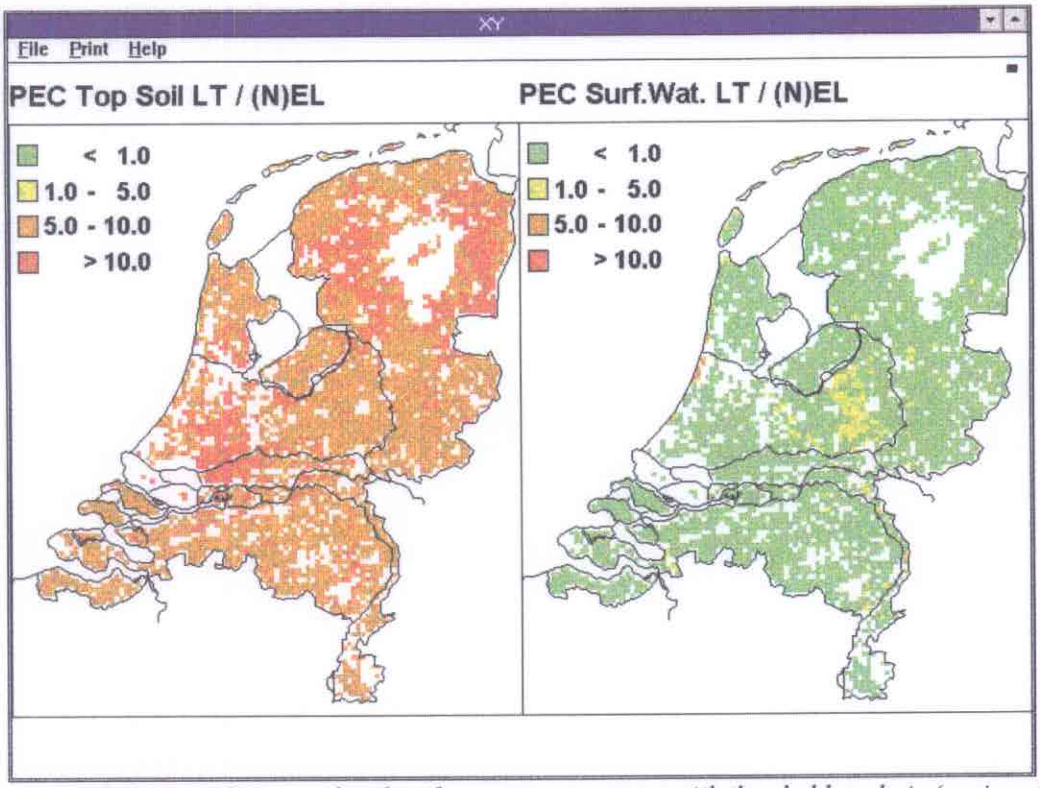


Figure 6.9. Risk ratios for top soil and surface water ecosystems with threshold analysis (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

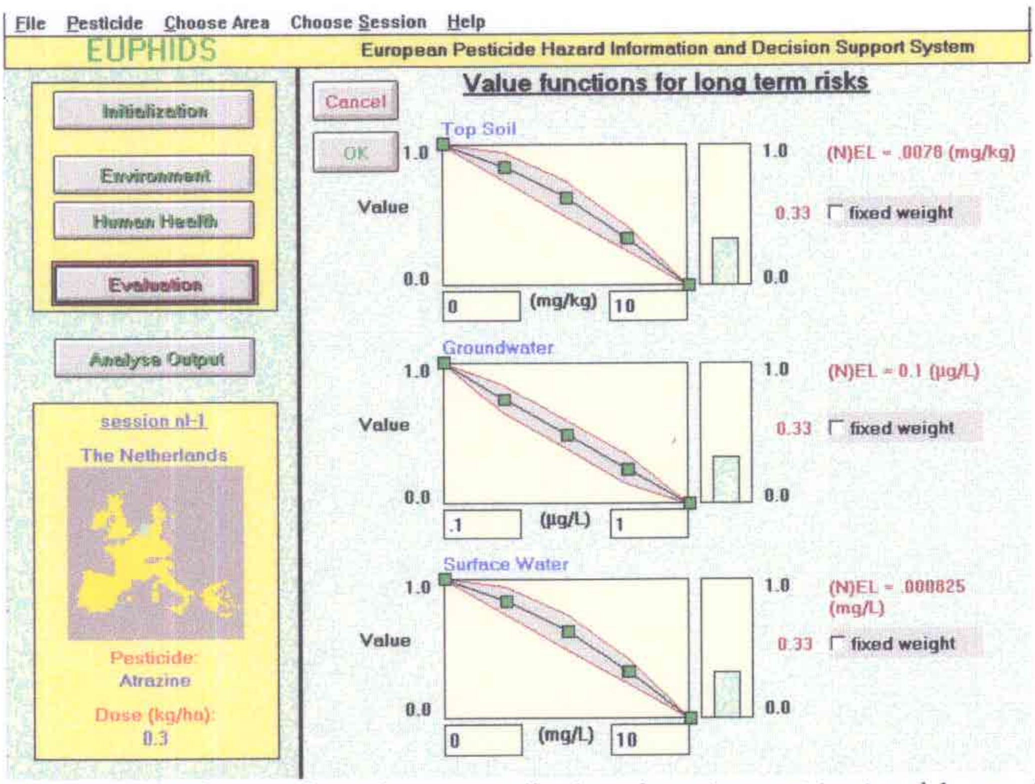


Figure 6.10. Value functions for evaluating overall risks to the environment (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

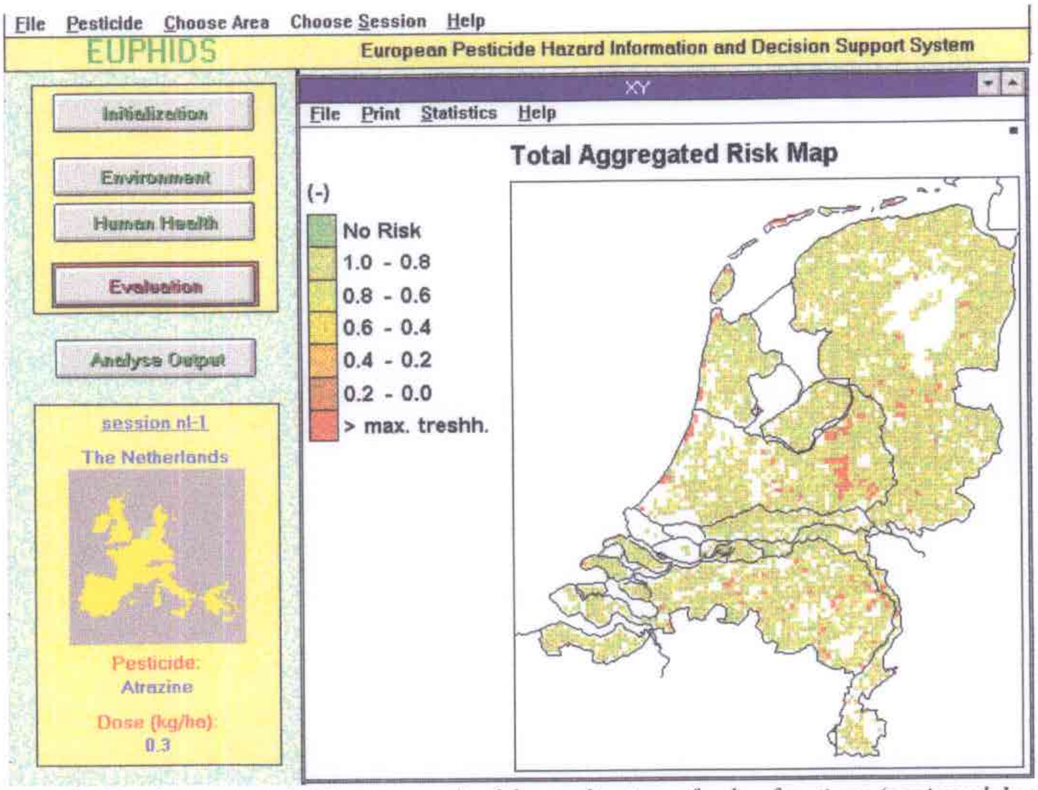


Figure 6.11. Total aggregated risk map, result of the application of value functions (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

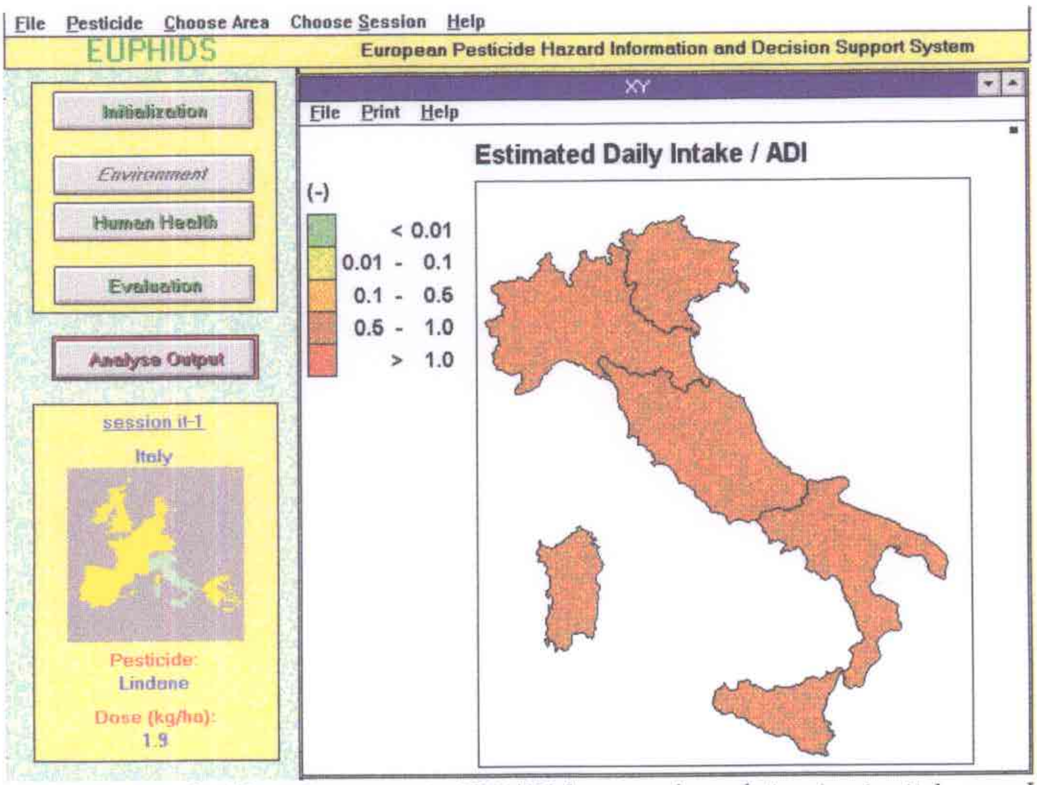


Figure 6.12. Human health evaluation: ratio EDI/ADI for general population (session it-1; area: Italy; pesticide Lindane; dose: 1.9 kg/ha).

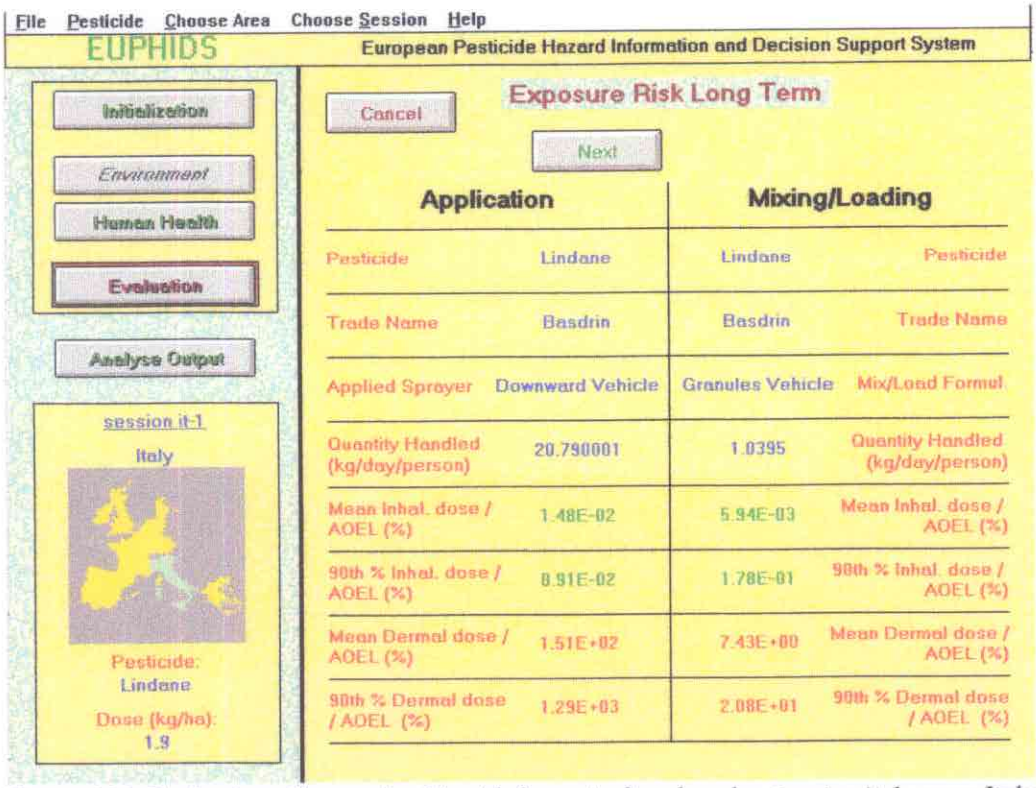


Figure 6.13. Evaluation of human health: risk for agricultural worker (session it-1; area: Italy; pesticide Lindane; dose: 1.9 kg/ha).

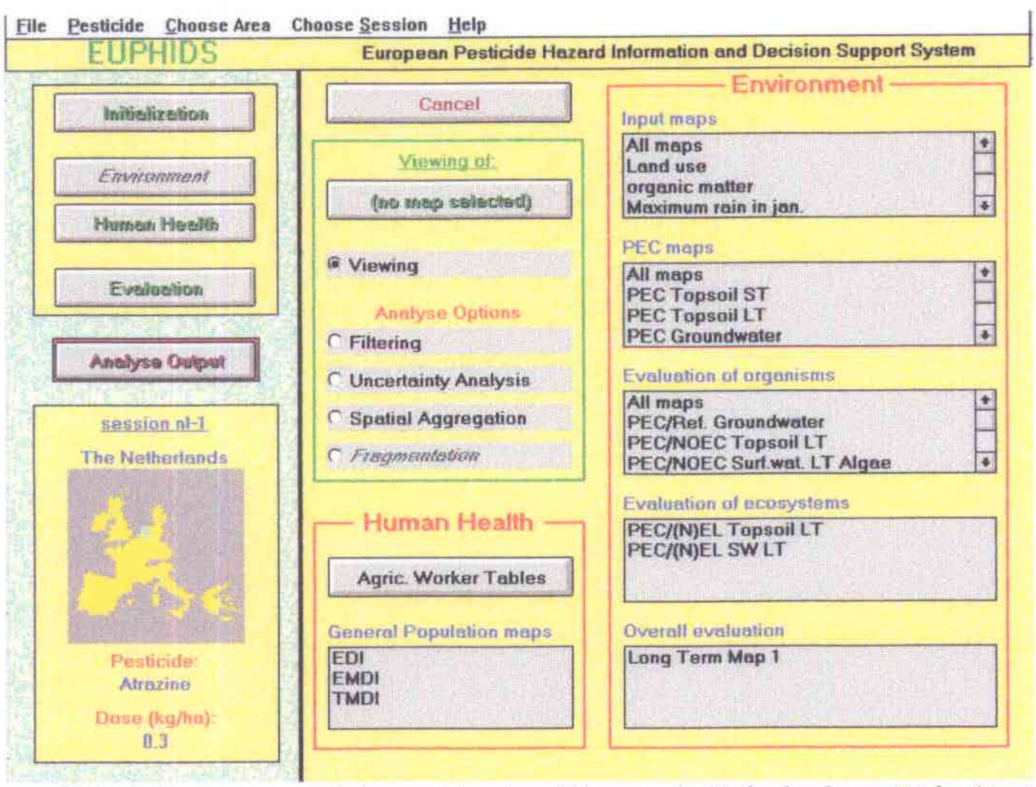


Figure 6.14. Analyse output: global screen (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

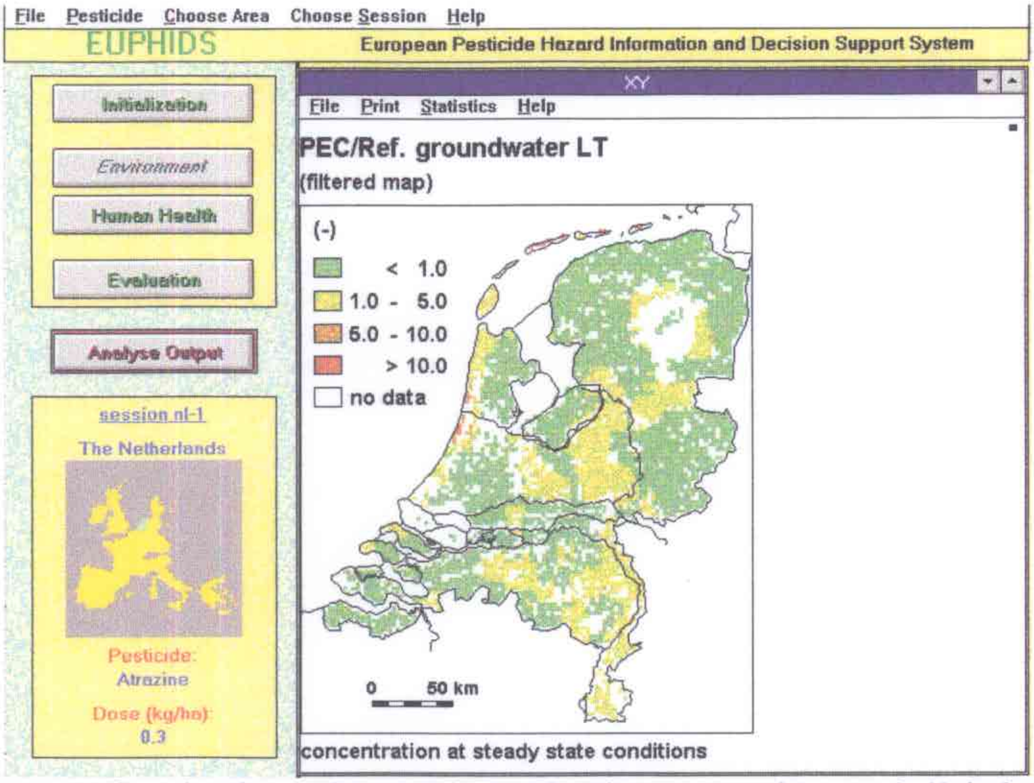


Figure 6.15. Spatial analysis; risk to groundwater: filtered map (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

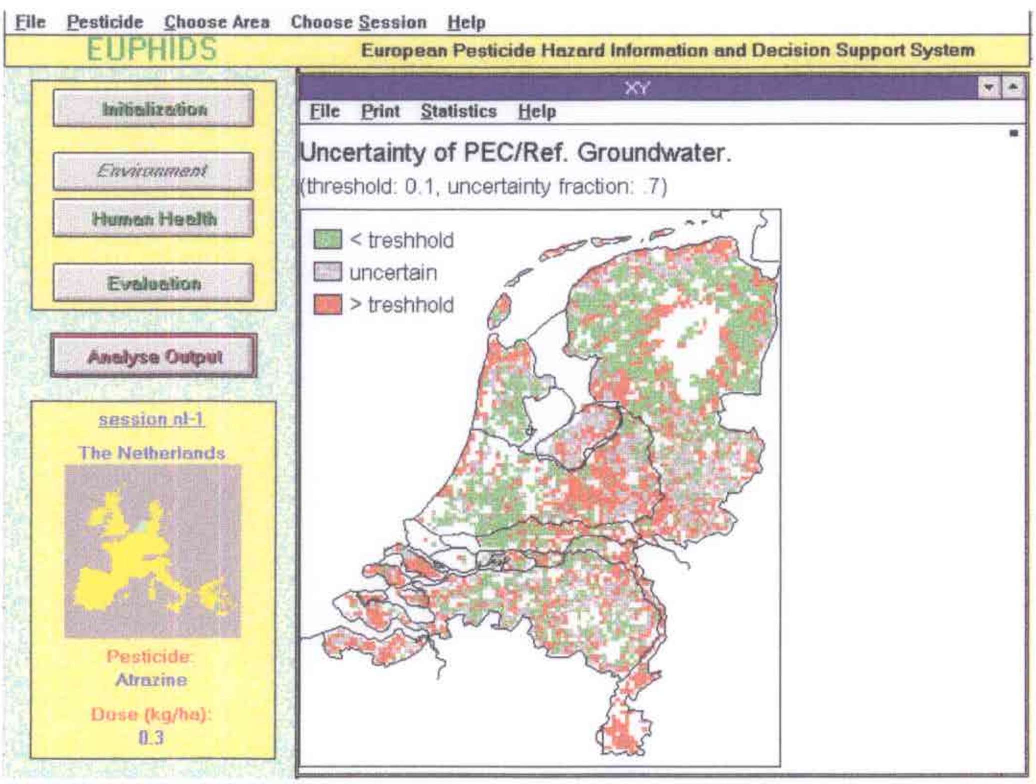


Figure 6.16. Spatial analysis; risk to groundwater: uncertainty in the PEC/reference risk ratio (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

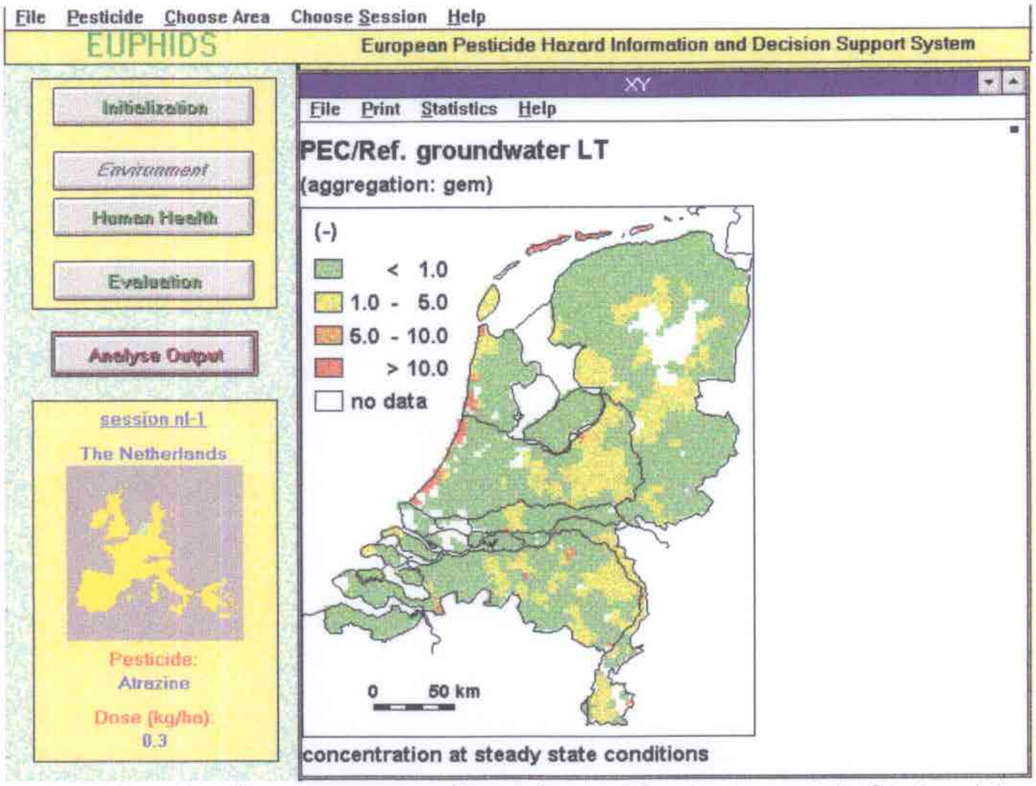


Figure 6.17. Spatial analysis; aggregation of groundwater risk ratios per municipality (gem.) (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

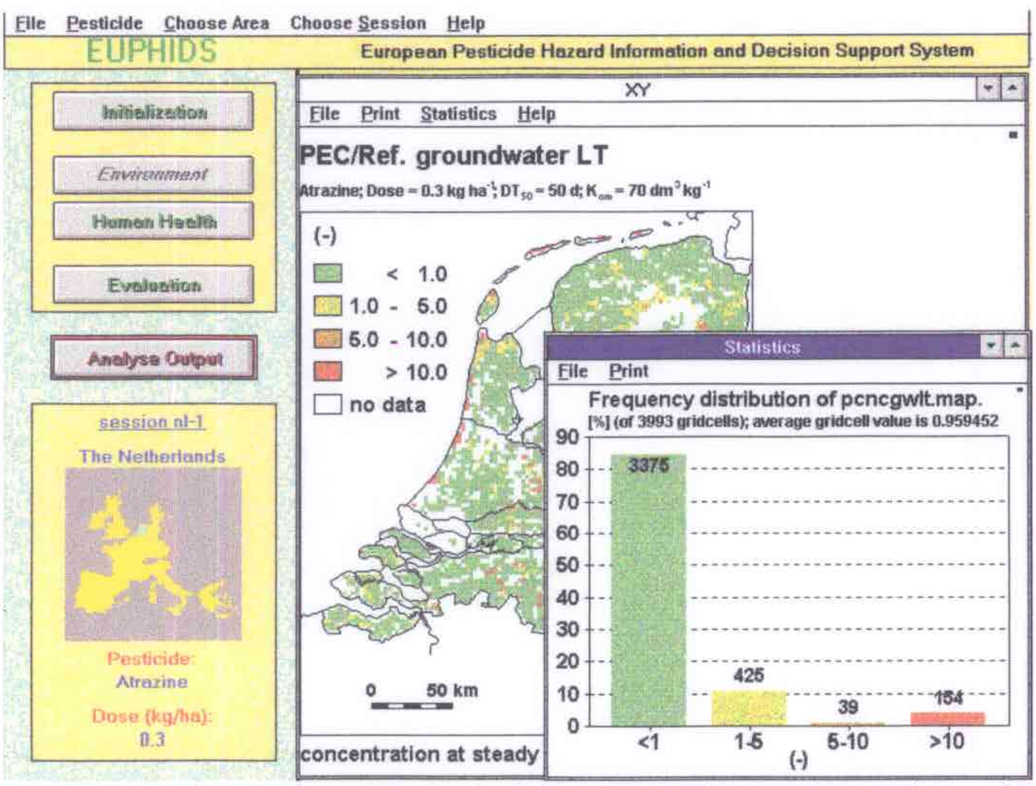


Figure 6.18. Statistical analysis: number of grid cells per classes in the groundwater risk map of Figure 6.8 (session nl-1; area: the Netherlands; pesticide: Atrazine; dose: 0.3 kg/ha).

7. Discussion

7.1. Ecotoxicological assessment and evaluation

The ecotoxicological exposure and risk assessment modules of EUPHIDS are based on broadly accepted methods like, e.g., scenario-approaches, exposure models and effect-assessment methods which also include the principles for the exposure and risk assessment as stated in the "Uniform Principles" (UP, Council-Directive 94/43/EC). This methodology is the scientifically undisputed approach to evaluate the pesticide risk from the ratio of the predicted environmental concentration and (extrapolated) toxicological information from tests with certain species. This approach is supplemented and extended by spatial data for environmental parameters provided by the GIS-environment included in the program. By combining pesticide related data and spatial variables, spatially differentiated PECs are obtained which in combination with the currently non-spatial (no-)effect levels ((N)EL) for organisms and ecosystems result in a spatial pesticide risk assessment. Information on differences in species sensitivity due to environmental conditions like edaphic parameters, water chemistry and climate could improve the spatial differentiation of risk very much, as well as toxicity data on other than the standard test organisms (i.e. species inhabiting particular regions or ecosystem types). Unfortunately such data were either not available or not as comprehensive and consistent that it could be used to model such spatial differences. However, to devise and implement an approach to account for spatial variance in species sensitivity is a challenging task for the further improvement of EUPHIDS.

It was considered as useful to extend the risk assessment module with further options beside the UP approach, including internationally recognised and acknowledged methods such as the EPA-method (EPA, 1984) or the sensitivity distribution method devised by Aldenberg and Slob (1993) which aim at risk assessment for ecosystems instead of checking risk for a number of species, as it is the scope of the UP. Beside the different subjects of the assessment procedures (ecosystems versus single species), the Aldenberg and Slob procedure offers additionally a new and appealing approach for toxicity data extrapolation based on mathematical considerations. Unfortunately, this method is yet hardly applicable for pesticide registration since at least 4 NOECs for organisms of different taxonomic groups should be available for each environmental compartment when applying the method. This means NOEC data for more species than the applicants are currently obliged to provide for the toxicity assessment of their products. Therefore the toxicity information from the dossier would need to be extended with data from additional sources. However, the different options for risk assessment offer a versatile and flexible toolbox both to conduct comparative risk evaluations by different methods or to adapt the assessment procedure for the solution of particular problems or questions. Additionally, this toolbox is appended by a further very useful functionality, the integration of risks for the environmental compartments (terrestrial, aquatic and groundwater) by the value function approach. This kind of integrated risk assessment provides a clearly defined, transparent and consistent method to get indications for the extent of pesticide risk posed simultaneously on the environment.

The approaches used for the estimation of predicted environmental concentrations (PECs) for the aquatic and terrestrial compartments and for groundwater are rather simple and, thus, reduce or neglect some real world parameters and processes having influence on fate of and exposure by plant protection products. Anyway, the principal and quantitatively important fate and exposure governing processes are of course included in the models. Therefore, this methodology for predicting environmental concentrations and environmental risk may not be suitable to correctly predict PECs and risk for any specific site but it is appropriate to identify and to rank regions (the size of which depends on the chosen scale) with respect to their vulnerability.

The reason for choosing or setting up models and scenarios as they are is, on the one hand, the limited availability of spatial and pesticide related data necessary to perform exposure and risk assessments with more sophisticated scenarios and models. On the other hand, it is the intended consistency of the assessment approach of EUPHIDS with the currently accepted and widely used conventional procedures. These conventional procedures are based on even more simple ((realistic) worst case) scenario assumptions and they additionally do not consider spatial variability of environmental conditions. Thus, the use of rather simple scenarios and models in EUPHIDS is no weak point of the system but the result of bringing two objectives into line: acceptance of the EUPHIDS approach by the competent authorities responsible for the admission of pesticides and operability of the system due to confinement of model and scenario architecture to available data. For plant protection products these are the physico-chemical and toxicity data which have to be delivered by the applicants. But also the availability of spatial data is limiting the set-up of whatever more complex models and scenarios. Thus, a better reflection of real world conditions in the course of modelling pesticide exposure, effects and risk requires, first of all, the availability of more and other data. This means to claim the investigation of more parameters as well as a higher resolution of available data in space and time such as - inter alia - species sensitivities related to regional environmental conditions or spatial variability of bioavailability. Data of the latter type could enable a spatial assessment of species sensitivity and, thus, improve the spatial differentiation and reliability of the ecotoxicological risk assessment.

Nonetheless, apart from data availability, there is still scope to improve the performance of the environmental models and scenario assumptions implemented in EUPHIDS in the sense of a more reliable and spatially more differentiated reflection of real world conditions.

For instance, the PEC calculation for surface waters could be improved by consideration of spatial variability in advective transport of water due to topographical conditions. Also a distinction between exposure in smaller (ditch) and larger water bodies (e.g. rivers, lakes) may be considered. This could include the use of available pesticide background concentrations. With respect to exposure of surface water by run-off, a distance decay function accounting for the drop down of pesticide concentration along with distance between treated field and water body still has to be implemented in the current calculation procedure. But it may also be figured out whether the currently used quantitative model based on expert judgement and empirically found equations should be replaced by other approaches like a more theoretically based description of the run-off process[1] or by a qualitative assessment of run-off probability and intensity[2]. Such a qualitative assessment procedure is not consistent with any of the other quantitative models in EUPHIDS currently used to calculate PECs. The approach is based on a scoring system for the relevant parameters and, thus, reflecting expert judgement. Therefore, it is to some extend similar to the risk assessment by value functions. Its main strength is to avoid some kind of quantitative pseudo accuracy for a process which, due to its nature, is hardly ascertainable by a quantitative description. A more detailed model for exposure in surface water, named TOXSWA, is elaborated in the Netherlands, and in future can be evaluated as an alternative.

In terms of a better reflection of pesticide application modes in EUPHIDS an option to choose between spring and fall applications for the assessment of leaching to groundwater should be implemented since groundwater contamination by a pesticide may depend on the time of its application. Moreover, the opportunity to calculate PECs for surface water and soil after repeated applications should also be considered as an important step to improve the flexibility and versatility of the system. A proposal how to tackle multiple pesticide applications in EUPHIDS already exists[3].

Rice cultivation gives rise to flooding of the agricultural land. For the calculation of leaching in these cases a solution is not yet foreseen. The same goes for irrigation, although this can rather easily be implemented by adding soil-climate-irrigation scenarios.

An improvement which is foreseen, is the temperature dependence of the biodegradation, which has impact on the long term calculated exposure in surface water. For exposure in soil and groundwater this has already been realised. Also influencing biodegradation is the moisture content of the soil. How this can be modelled in scenario type calculations is not yet clear.

Another improvement which is necessary, but for which a widely accepted model is not yet available, is the problem of preferential flow. But before implementing preferential flow, its impact on the total leaching should be evaluated.

For the assessment of risk to the terrestrial environment it can be clearly stated that more species and components than those currently considered (earthworms) need to be included in the EUPHIDS program. All terrestrial species currently being tested for the purpose of pesticide risk assessment must, to a high extent, already be protected from adverse effects under the conditions of a treated field. Therefore, an exposure and effects analysis for treated fields is sufficient to assess risk to the entire terrestrial environment as long as no more stringent safety margins for the non-target terrestrial environment exist. To be able to conduct the respective exposure and risk estimates, appropriate field scenarios for PECs as well as for species food uptake have to be set up. A proposal for such scenarios already exists[4] but the respective scenarios still have to be included in EUPHIDS.

[1] See appendix A8 “Alternative description of runoff decay“
[2] See appendix A5 “Qualitative assessment of run-off probability and intensity“
[3] See appendix A6 “Multiple applications“
[4] See appendix A7 “Estimation of PECs and pesticide risks for organisms of the terrestrial environment“

Formulations of pesticides have not been taken into consideration. The importance of this aspect is mostly dependent on the time scale of the assessment. For example, when simulating pesticide leaching to groundwater, which usually takes one or more years, the formulation does not have significant influence. On the other hand, short term processes as spraydrift will be influenced by the pesticide formulation but the present knowledge on the functions is still too poor to implement validated models into EUPHIDS. Moreover, drift and interception tables implicitly take formulations into account as the data were gathered from experiments in which formulations were used.

Combinations of pesticides were also not taken into consideration in the ecotoxicological assessment. For the estimation of exposure concentration (PEC) the influence of combinations is rather low. Of course, this is not true for the estimation of the toxicity in the environment where non-additional effects often have been observed. But again, too few experimental data are available in this field to implement models into EUPHIDS. As first approximation of the risk evaluation of a combination of pesticides, after evaluating the individual components, the individual results might be combined (added).

7.2. Human toxicological assessment and evaluation

The assessment of human health risk for exposure to chemicals is a complex matter for every chemical substance, but even more so for pesticides due to the specific conditions of their use. The procedure implemented in EUPHIDS takes into consideration the two main targets - agricultural workers and the general population - but does not consider other minor aspects, such as the "bystander" exposure, exposure of workers due to re-entry in treated crop areas, exposure in greenhouses, and general population exposure due to spray drifts. In addition other exposure conditions that may deserve a special treatment, such as aerial application, have not been taken into consideration due to the limited time available to the project.

In the future all these aspects could be dealt with by including new specific modules in the system. For the sake of simplicity, also distant aerial diffusion due to evaporation or transport of air drifts have been omitted. This mode of exposure can be relevant particularly when assessing fumigants or highly volatile substances and its inclusion in the system is desirable in the future.

As concerns the capabilities of the present system, one of the first additions to be made concerns the choice of the model to calculate the exposure level for the agricultural worker. As soon as there is sufficient consensus on one European model, this model should be incorporated.

Another desirable addition concerns the possibility to differentiate between sensitive groups of the population, in particular infants and children. These groups have dietary requirements different from those of the adult population and need a specific dietary database. In addition, they may be hyper-susceptible to the toxic action of chemicals and a specific ADI may be indicated.

The procedure adopted for the human health risk assessment in EUPHIDS finds global consensus in the scientific community. There are of course areas of uncertainty both in the exposure part and in the toxicity assessment part, but no other methods can reliably be used until new substantial knowledge is developed in the basic sciences from which the procedure stems. The most debated issues in the procedure (selection of the appropriate NOEL, selection of the Safety Factor value, etc.) have been treated in a flexible way enabling the user to adopt default values or, when felt appropriate, to introduce other values.

In addition to the more consolidated methods for assessment of long-term effects (usually the crucial issue to the rejection of the pesticides), EUPHIDS also provides a specific module for the description of the acute effect risk (or margin of safety). This module has been designed to help the users to assess the need for recommending special care in handling the compounds and/or personal protective devices particularly for those pesticides with high acute toxicity and relatively low long-term toxicity.

Pesticides are frequently used as formulations in combination with other compounds, often considered "inert". When the toxicity of an active ingredient has been determined, the investigation on formulation is generally restricted to acute studies. Combination of pesticides in one formulation may need characterisation of long-term toxicity.

No single approach exists to assess adverse effects of mixtures. Since this issue is very complex and only limited toxicological data are available on tests of mixtures, it is of extreme importance to use experience and knowledge in a flexible way. In general, toxicity assessment of mixtures is not essentially different from that performed for individual compounds, although special considerations should be given to the stability of the mixture and the possible interactions (chemical, metabolic, and toxicological) between components. In the future EUPHIDS could develop special techniques for integrating information on mixtures, although there is not a general consensus on their adoption.

7.3. System development

Apart from amendments with respect to better description of certain exposure pathways and necessities for additional switches etc. (e.g. with/without advection in surface water, spring or fall application for leaching) the following suggestions are made to improve the performance of the decision support system:

- saving of individual maps
- comparison of maps (e.g. sensitivity maps, PESTRAS and PELMO maps)
- comparison of maps for different pesticides (ranking of pesticides)
- improved output environment (according to user specifications).

Moreover the system should be improved to gain in robustness.

7.4. General discussion

The achievement of harmonisation among the European countries and the national groups of experts in the admission of pesticides is one of the most relevant aims of the directive 91/414. To this purpose the Uniform Principles have set general criteria which define the relevant targets and the general procedures of assessment. It has to be noted, however, that the Uniform Principles do not provide detailed methods and procedures for the quantitative risk assessment of each relevant target and, in particular, there is no specification of the methods by which the assessment can be linked to the specific characteristics of each area.

EUPHIDS has filled this gap by adopting scientifically sound models of prediction for phenomena such as leaching, run-off, spray-drift, exposure of the operators and exposure of the general population through the diet. For each of these phenomena, algorithms have been developed that allow calculation and quantification of the dose delivered to the targets. Moreover the models have been applied in such a way that the specific features of each environment can be taken into account at various scales of work (continental, national, local) and the spatial variation of the assessment can be described with appropriate maps.

In the future EUPHIDS may be further enriched by adding new alternative models for the assessment of each process and leaving to the user the selection among the preferred methodological option. In this respect EUPHIDS is an open and flexible system.

So far EUPHIDS is structured to provide only the risk evaluation of pesticide use. In the future it could be further expanded to include other aspects which are very important in the whole process of the risk/benefit analysis. For example, new modules could be added for the assessment of efficacy of the use of pesticides and the estimation of the economic benefits expected to the agricultural production. The development of these expansions requires disciplinary expertise that goes beyond the research group that has developed EUPHIDS; however it has to be remarked that EUPHIDS has been designed as an open, flexible system that can be easily completed or amended, due to its modular form.

While highlighting the merits of EUPHIDS as a decision support tool, its limitations and proper use have also to be discussed. Firstly EUPHIDS is intended to support the decision process, but in no way can be seen as a system replacing its user in his/her function as assessor and decision maker; in fact, the user has to set the functionality of the system by providing input data, selecting appropriate values for many variables, and by choosing among options for calculation according to the specific nature of the task to be accomplished. Thus the result of the assessment, although aiming at objectivity and transparency, cannot avoid to be strongly influenced by the assumptions and the selections of the user. This is particularly important in the final module of the system where the individual evaluations on the ecosystem targets are synthesised into a single value by means of the value-function method. This approach has the advantage of providing a highly integrated, concise result sometimes very useful for comparative evaluations and for non-technical decision makers, but of course "conceals" several subjective assumptions to the final recipient of the product.

A second important aspect of EUPHIDS is its prototype character. It is clear that in order to be able to use EUPHIDS everywhere in Europe and at scales varying from continental to local (that is geographic scales of 1:1,000,000 to 1:10,000), an enormous amount of spatial data on the area are necessary. Within the frame of this three-year project it has only been possible to include in the system geographic data pertaining to some areas for demonstration of the capability of the system; this further data collection and acquisition is needed for a full implementation of the system. Another major obstacle for the development of a geographic decision support system lies in the availability and confidentiality of most of the existing data on the environment. While the user generally will have access to the toxicological data provided by the industry files for registration or from the open literature, the geographic data, in particular land use maps, organic carbon content of the soil, etc., are difficult to obtain and cannot be circulated in such a way that they can be reproduced by any user. It is hoped that in the future, also by action of the European Commission, such data are made more easily available at the international and national level.

Besides data availability, the use of EUPHIDS also requires an information infrastructure combined with some basic skills in the disciplines involved in the risk-assessment process and in the use of elementary geographic information systems. Therefore the EUPHIDS user should become familiar with the technical procedures involved in the use of geographical information systems.

The user, with the necessary organisation, will be able to reproduce reliable evaluations, print thematic maps, add new substances in additions, to these now included for demonstration, and, to some extent, personalise EUPHIDS with the inclusion of the environment data of his/her interest. By acquiring familiarity with the functionality of EUPHIDS and having direct knowledge of the quality of data provided to it, the user will also be able to interpret the results properly, understanding the informative power of EUPHIDS at the various scales of work.

Due to the nature of this system, it has to be realised that the sensitivity of the analysis is determined by the scale at which the data are imputed, the method of data aggregation, and the scale at which they are released. Ideally the evaluation at the different scales should be the same or, at least, consistent; in practice this depends on whether or not the same data are imputed at various scales and the data aggregation process does not produce masking distortions.

In spite of the limits present in EUPHIDS, this research project has demonstrated that a new way can be trod in the development of a decision support system for the admission of pesticides. The originality of the products lies in the integration of different disciplinary expertise and the combination of toxicology, ecotoxicology, environmental sciences, and information and social sciences into a single, uniform tool. The decision maker thus can receive information on risk (what) and its temporal and spatial variation (when and where). In the future it would be of great interest to explore the use of EUPHIDS also to plan the surveillance programmes required by the directive 91/414 and to integrate the monitoring results for a continuous re-evaluation of these substances.

8. Conclusions and recommendations

8.1. Conclusions

The spatial component of risk assessment is of fundamental importance for pesticide admission. In this way specific, instead of generic, policy measures can be taken. Therefore, the next generation of our information infrastructures needs to take into account the spatial component.

An innovative concept has been developed to integrate data collection, data analysis, data presentation and evaluation procedures. EUPHIDS, as a system, represents the operative tool of this innovative concept.

This decision support system is the first or one of the first considering the spatial scale and is built upon risk assessment schemes including the models already developed and used in other frameworks: in the Netherlands, Germany, Italy, etc..

The DSS-module is an open, flexible system and can easily be loaded with state-of-the-art knowledge (data, models, rules) to provide the decision-maker with the information needed, according to the Uniform Principles.
At this moment only a part of the UP (the risk assessment part) and their aspects with a spatial relation have been considered.

The risk assessment as well as the evaluation models used in EUPHIDS represent the state-of-the-art models available at this moment, also in relation to data availability (process as well as pesticide parameters).

Consistency of data, data quality and data availability are the main aspects for the success of decision support systems with a spatial component. Non-spatial decision making is easier, but neglects the regional differences.

Care should be taken in interpreting results of the EUPHIDS calculations; the use of models provides an estimation, but remains a prediction in which all uncertainties should be considered. At least EUPHIDS offers a clear insight in the decision information - the risks - and is a very valuable tool in comparing risks in countries, regions, and of different pesticides in a uniform and reproducible way.

8.2. Recommendations

As a powerful tool to support the decision makers, it is necessary to discuss the benefits and the concept of the system with the EU-decision-makers (DG V, VI, XI, the Standing Committee) and the national committees; moreover, information is necessary on the need for aggregation of information, value functions, uncertainties, and "realistic" worst case scenarios.

Only state-of-the-art models, "validated" should be incorporated; these models should also meet the data availability (on pesticides and processes). If applied in the EU decision-making process it should contain the models agreed upon in the EU (FOCUS group).

A lot of improvements, suggested and sometimes already available, should be built in the system to extend the system towards a fully operational DSS.

The system should at least be completed with other risk assessment aspects related to the terrestrial environment (e.g. birds, mammals, and honey bees), preferably also considering spatial scale.

New, improved, more detailed models (for leaching, surface water PEC calculation) should be considered, but always related to data availability (on the short and the long term).

The system should make it possible to present the results of the various models (on the same subject) and to make a comparison possible (provides information on variability, uncertainties etc.).

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APPENDICES

This set of Appendices is divided into three parts. The first part collects all the reference material used for the development of EUPHIDS. The second part described the future developments of EUPHIDS for which there is already an extensive analytical treatment but which are not yet implemented. The third part lists the publications and presentations of EUPHIDS as a part of the dissemination of results of the project.

PART ONE: Reference information.

A1: Definitions and abbreviations. Contains the lists of all abbreviations and definitions of terms and acronyms used in the text.
A2: Value functions. Describes the assessment of value functions and the rationale for the choices made in Chapter 3.
A3: European spatial scenarios for pesticide leaching. This part describes the definition and computation of spatial scenarios for leaching in Europe, Germany, The Netherlands and Italy.
A4: Meta information on spatial data. This appendix lists all the maps used as input in EUPHIDS. It describes the main attributes of the map, the characteristics of the geographical information included together with the source of the information and the processing necessary to interface the information with EUPHIDS.

PART TWO: Future developments.

A5: Qualitative assessment of run-off probability and intensity. Contains an alternative treatment of the run-off event on the basis of qualitative judgements and score classification.
A6: Multiple applications. Introduces the formulas for the calculation of concentrations of pesticide in soil and surface water as a result of multiple applications.
A7: Estimation of PEC and pesticide risks for organisms of the terrestrial environment. Describes the procedures to compute the exposure to terrestrial ecosystems such as birds and vertebrates.
A8: Alternative description of run-off decay. This part provides and enhanced version of the run-off decay calculation models.

PART THREE: Dissemination of results.

A9: Publications and presentations. Lists the publications and presentations made during the development of EUPHIDS by the project partners.

PART ONE: Reference material

A1. Definitions and abbreviations

ADI	Acceptable Daily Intake
AOEL	Acceptable Operator Exposure Level
API	Agricultural Product Residue, the pesticide content of an agricultural product
DT50	Transformation half-lifetime. The time necessary to transform 50% of a compound in the compartment considered - soil or surface water.
DV	average Diet Value of a food commodity consumed per capita.
DWC	Drinking Water Consumption, the amount of water consumed per capita per day
EC50	Median effective Concentration in an environmental medium expected to produce a certain effect in 50% of organisms in a given population under a defined set of conditions.
ED	External Dose, the amount of pesticide residue that reaches the skin or is inhaled per kg handled or applied.
EDI	Estimated Daily Intake, the best estimate of the daily intake of a pesticide residue, taking into account besides EP and TPC also the Market Share (MS) of the pesticide in all crops and actually observed concentrations of the pesticide in the crop.
EMDI	Estimated Maximum Daily Intake, a prediction of the maximum daily intake of a pesticide residue taking into account the Edible Portion (EP) of each food commodity and altering of the concentration due to food processing.
EP	Edible Portion, that part of food that actually is consumed.
EUPHIDS	EUropean Pesticide Hazard Information and Decision support System. The system described in this report.
HA	Handled Amount, the amount of a pesticide handled by the agricultural worker per day
IARC	International Agency for Research on Cancer
ID	Internal Dose, the amount of pesticide absorbed per day by a person working in agriculture
Kom	Sorption equilibrium constant of a compound solved in the liquid phase and sorbed to the solid organic matter phase.
Koc	Sorption equilibrium constant of a compound solved in the liquid phase and sorbed to the solid organic carbon phase.
LD50	Median lethal Dose expected to kill 50% of organisms in a given population under a defined set of conditions.
LC50	Median lethal Concentration in an environmental medium expected to kill 50% of organisms in a given population under a defined set of conditions.
MOLD	Minimum Observed Lethal Dose
MRC	Maximum Residue Concentration, the maximum allowed concentration of a pesticide in drinking water, currently 0.1 μ/l according to Directive 222280/778/EEC
MRL	Maximum Residue Level. The maximum allowable residue concentration of a pesticide in food commodities.

MS	Market Share, the proportion of a crop treated with a given pesticide.
(N)EL	(No)-Effect Level. That concentration or intake level that is supposed to have (no) adverse effects on man or environment.
NOAEL	No Observed Adverse Effect Level
NOEL	No Observed Effect Level
PEC	Predicted Environmental Concentration. Concentration of a pesticide in an environmental compartment as predicted by a calculation method. In EUPHIDS in general scenario type calculations are performed.
PELMO	PEsticide Leaching MOdel. German simulation model for calculating leaching of pesticides to groundwater.
PESTRAS	PESTicide TRansport ASsessment model. Dutch simulation model for calculating leaching of pesticides to groundwater.
PIEC	Predicted Initial Environmental Concentration. A PEC calculated upon entrance of a compound in the compartment.
PPC	Potability Process Coefficient, parameter defining the alteration of the concentration of a pesticide residue in water due to purification of the water. This PPC may vary spatially due to different processing techniques.
Q*	Unit Cancer Risk
Risk Characterisation	Ratio between the absorbed dose and the NOEL
SF	Safety Factor
SWR	Source Water Residue concentration, the predicted or measured concentration of a pesticide in water that is used for the production of drinking water
TF	Time Factor
TMDI	Theoretical Maximum Daily Intake. Estimate of the dietary intake (per person), based on the assumption of residue concentrations in the food on the market equal to the maximum limit values (MRL) and the average daily per capita consumption of each food commodity for which an MRL has to be established. The TMDI is expressed in milligram of residue per person.
TPC	Transformation Process Coefficient, parameter accounting for the alteration of a concentration of a pesticide residue due to processing the food.

A2. Value functions

A2.1. Assessment of value functions

Value functions represent expert judgement on the relative risks between the risk threshold L and H as defined in Chapter 3. The assessment of value functions and weights requires ad-hoc procedures to interview experts and to assess their knowledge. There are four basic points which require careful analysis for the value function assessment:

1. the selection of the limit scores and profiles (L,H for each compartment);
2. the interpretation of value functions;
3. the assessment of the shape of the value function;
4. the assessment of the weights.

A2.2. Selection of the limit profiles

In Chapter 3, the levels (N)EL and 10*(N)EL have been used as the range of PECs for the value function domain. This is not the only possible choice. In general, the value function model requires two end points, a low level L and a high level H, between which to anchor the evaluation. The only requirement to these points is that they have to represent two clear limit situations:

- PECs lower that L for any compartment should represent a threshold below which there is sufficient certainty that adverse effects do not occur. In this range there is no need to perform additional risk analysis and thus should be a natural lower bound for a value function.
- PECs higher than H for any compartment should not be taken into account as they highlight an unacceptable risk for the environment. In this range there is no need to perform additional risk analysis and thus H is the upper bound for a value function.

Due to the definition of (N)EL (cf. Appendix A1), the selection of L=(N)EL is rather natural in this context. On the contrary, the selection of H is less straightforward. It requires knowledge on the effects associate to H but also a judgement on the acceptability of the effects. This is an important point: any selection of the level H has to involve human judgement as there is no factual information which states that a certain effect is, or is not, acceptable for the environment.

The rationale for choosing H=10*(N)EL is linked to the EPA method for computing the (N)EL at the ecosystem level. The ecosystem (N)EL is calculated as the lowest NOEC available multiplied by a safety factor k: (N)EL = k*$NOEC_{min}$. This safety factor is equal to ten if three or more different NOECs are available for prescribed test species. In such a case, (N)EL=0.1*$NOEC_{min}$. As the test species are selected in order to span the ecosystem response to the pesticide, it is acceptable to say that the lowest NOEC is a good indicator or the most sensitive range of species in the ecosystem. PECs lower that (N)EL(=0.1*$NOEC_{min}$) are most likely to show no effects for the ecosystem, while PECs between (N)EL and 10*(N)EL(=$NOEC_{min}$) may affect only species more sensitive than those tested. By exceeding the 10*(N)EL (=$NOEC_{min}$) we reach the point at which the most sensitive species among those tested is affected with certainty and thus significant adverse environmental effects occur.

This approach relies on the EPA definition of (N)EL and requires at least three test species which justify the safety factor of ten. Given the requirements of the Uniform Principles, this seems an acceptable condition. In situations where this is not the case, the reasoning could be extrapolated. H can still be fixed at 10*(N)EL, regardless of the method used to compute (N)EL but in such a case it more complicated to relate it to a precise effect threshold. In such a case it is convenient to consider H as a reference limit used to frame the evaluation and make explicit an upper bound for the PECs to be analysed.

The choice of H=10*(N)EL might be applied to long and short term evaluations retaining the same interpretation. It should be noted, however, that other choices could be made. As an example, short term evaluations might require to span a larger range of effects, in which case H=10*(N)EL might be too restrictive. A possible solution for short term effects is to enlarge the evaluation range and to fix H at the lowest available LC_{50} level: H=min $\{LC_{50}\}$. The meaning of H in this context is that of a relaxed upper bound which could be used to take into account severe acute effects.

In short, in EUPHIDS the following l and H levels are used:

LONG TERM:	$L=(N)EL_{LT}$;
	$H=10*(N)EL_{LT}$;
SHORT TERM:	$L=(N)EL_{ST}$;
	$H=10*(N)EL_{ST}$.

A2.3. Interpretation of unidimensional value functions.

Unidimensional value functions are attached to each compartment separately. Their interpretation is made easier if they are compared to risk thresholds functions and to the dose-effect functions. Figure A2.1 shows an hypothetical dose-effect curve for an ecosystem[1] and two different threshold levels: (N)EL and 10*(N)EL. The part of the curve between these two levels is enlarged to show the relationship between dose-effect function, value function and risk thresholds.

For decision making purposes, the thresholds can be considered as step-wise value functions which only distinguish between a good level (value=1) and a bad level (value=0). The ideal value function, on the other hand, would represent the actual relationship between doses and effects. In such a case, the value function would simply be the complementary of effects rescaled into the [0-1] interval.

The (N)EL threshold is the most restrictive value function. If (N)EL is defined according to the EPA method, the (N)EL threshold serves to discard all PECs not at least 10 times lower than the lowest known effect threshold ($NOEC_{min}$). At the other extreme, the 10*(N)EL threshold does not accept PECs higher than the lowest known effect threshold ($NOEC_{min}$). They correspond to two opposed strategies. However, the intermediate zone

[1] A dose-effect curve at the ecosystem level could be the cumulative sensitivity distribution. In that case the effects would be the number of species affected by the PEC dose (cf. Aldenberg and Slob, 1993).

in which detailed effect evaluation determines the acceptability of the risk profiles cannot be assessed in this setting. The value function represents a flexible strategy which shows a smooth progression of effects between the thresholds. The natural shape of the curve is determined by the dose-effect function. In this sense it overrules the threshold evaluation introducing explicitly the relationship between dose and effects into the process.

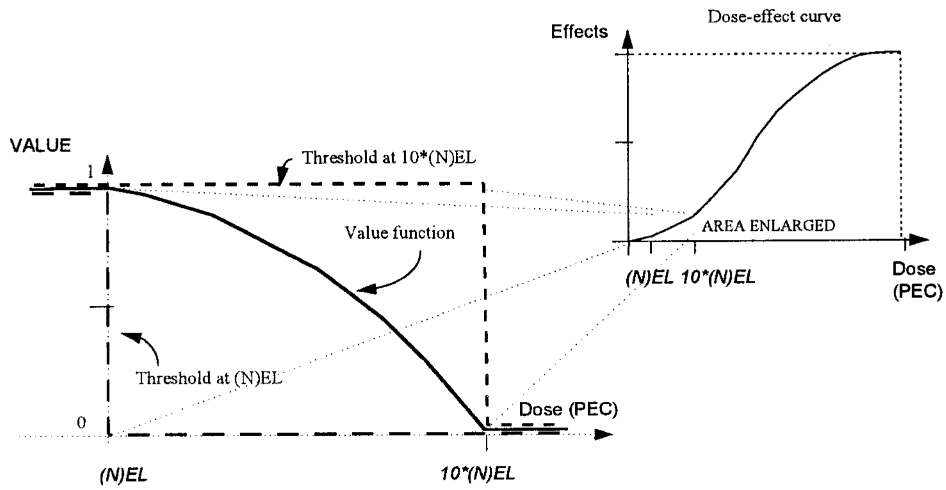

Figure A2.1. Value function and threshold functions within the range (N)EL, 10(N)EL.*

A2.4. Assessment of unidimensional value functions

The shape of the value function is straightforward if the dose-effect curve at the ecosystem level is known. As this is not the case, the shape of the curve has to extrapolated from available knowledge and expert judgement. Qualitative restrictions on the curve shape, however, are possible in most cases.

Given the interpretation of L and H levels and as it can be noted from Figure A2.1, the evaluation range for the value function is concentrated in the lower part of the dose-effect curve, well below the inflection point. This allows the assumption that the curve is concave and that the corresponding value function convex. Therefore the value curve has to be contained in the dotted area of . The curve can be further specified by asking expert judgement on the expected range of values (effects) of some intermediate points as shown in Figure A2.2. This would specify a value region and pose further limits to the curve. The final value function could simply be the mean curve if the value region is narrow. Otherwise, more sophisticated assessment techniques can be used to gather more expert judgements and lead to the final curve (see Beinat, 1995). It is worth noting that through appropriate techniques this expert assessment can be based on qualitative and imprecise responses only. In most cases few responses are sufficient to constraint the value region either to a single curve or to a very narrow set.

It should always be recognised that value functions are only approximations of dose-effect functions. They do not substitute missing toxicological data and do not overcome the lack of proper and detailed dose-effect functions. They structure available data and best expert judgement in such a way that risk assessment can be made transparent and reliable giving the decision maker a logical framework for effects appraisal.

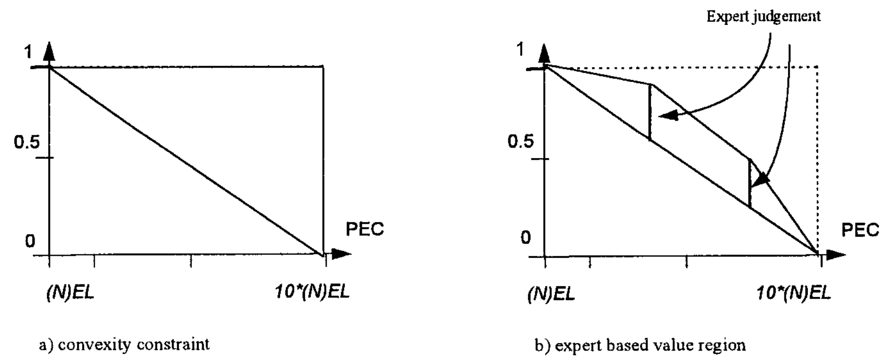

Figure A2.2. Shape constraints for the value functions

A2.5. Assessment of weight

Weights are used to aggregate value functions across compartments and lead to an overall value model. Each compartment is attached a weight which represent the relevance of its risks compared to the other compartments. More precisely, the weight of a compartment is the importance of the environmental effect attached to its H level compared to the H levels of the other categories.

Weighs depend on two pieces of information. First, the information on the actual expected effect of the H level; second, on the priority attached to this effect. Weights can be equal if the H level has the same interpretation across compartment and there is no need to highlight specific compartments. Differential weights can be used to stress some compartment effects. A typical example is the need of highlighting different protection levels for aquatic or terrestrial ecosystems in locations with different environmental qualities.

A2.6. Remarks

The value function technique provides the support for evaluating risk profiles which are difficult to assess only on the basis of threshold analysis. Value functions can be seen as approximations and local substitutes of unavailable dose-effect curves at the ecosystem level. They accommodate for the available laboratory evidence and provide a well structure frame for expert judgement. The assessment of value functions requires some insight into several pieces of information. It should be noted , however, that this kind of information (dose-effect curves, weights of evaluation categories, aggregation rule for synthesising risks) is necessary and implicitly introduced along risk assessment in any case, with or without value functions. The difference is that in the implicit process there is no mention of the information know, its uncertainty, the rules used and the link between data and risk evaluation. By using value functions we introduce these pieces of information explicitly. The extra effort required for the assessment has the advantage of increasing substantially the process in terms of structure, clarity and transparency.

A3. Spatial scenarios for pesticide leaching

A3.1. European scenarios

Scenario selection is based on a sensitivity analysis of the pesticide simulation model PESTRAS. From this analysis (Swartjes et al., 1993) it is clear that sensitivities are rather complex. In general, one can state that leaching is influenced by (in descending order of sensitivity):

Pesticide parameters on sorption and transformation
Climate parameters on temperature and precipitation
Soil hydraulic parameters
Crop parameters

The pesticide parameters can be varied in the EUPHIDS program and are therefore not part of the scenario. Sorption is very dependent on organic matter content of the soil, which is available for each grid cell and therefore also not part of the scenario. In the map of Europe (see Chapter 3, Figure 3.6), the continent was divided into several scenarios based on climatic differences. The climatic regions were chosen on the basis of combinations of precipitation excess and temperature(annual averages). This figure was obtained from the climatic map of the PANSOE project containing precipitation excess and temperature. In ARC/INFO, these parameters were combined using a Boolean AND statement to obtain scenarios. Subsequently, the map was generalised to specify the dominant scenario which leads to areas indicates in the map. The next step was to assign dominant landuse, organic matter content and soil type to each area. This was done by comparing the relevant maps with the scenario map and to determine the dominant class within a climatic area. The relevant maps were: the landuse map of Europe used within the PANSOE project, the soil organic matter map of Europe, based on the FAO soil map, and the CORINE soil map based on the FAO soil map.

Leaching of pesticides was calculated by assuming, that the conditions, determined for the scenario regions are representative for each entire region. Precipitation data were obtained from The Netherlands and Italy. With a transfer function, the daily data for the other regions were calculated:

$$P_{station} = P_{reference} * \frac{\overline{P}_{station}}{\overline{P}_{reference}} \quad \text{and similarly} \quad T_{station} = T_{reference} * \frac{\overline{T}_{station}}{\overline{T}_{reference}}$$

In which:

$P_{station}$ = daily precipitation value (mm) of a station in a scenario region
$P_{reference}$ = daily precipitation value (mm) of a station for which data are available
$\overline{P}_{station}$ = (long year) annual average precipitation for the weather station in the scenario region considered
$\overline{P}_{reference}$ = (long year) annual average precipitation for the weather station for which data are available.
$T_{station}$ = daily temperature (°C) of the station in a scenario region
$T_{reference}$ = daily temperature of the station for which data are available

$\overline{T}_{station}$ = (long year) annual average temperature for the weather station in the scenario region

$\overline{T}_{reference}$ = (long year) annual average temperature of the station for which data are available.

Scenarios 1,2,3,7 and 8 are based on Italian data; scenarios 5 and 6 are based on Dutch data; scenario 4 is based on an average of Dutch and Italian scenarios. In order to calculate evaporation, PESTRAS requires global radiation data. Since these data are mainly dependent on latitude, scenarios 1,2,3,7, and 8 are assumed equal, as is the case with scenarios 5 and 6. Differences in evaporation are assumed to be caused by temperature differences. Scenario number 4 is again an average of Dutch and Italian data. The following table gives the definition of the scenarios.

Table A3.1. Definition of the European scenario regions.

	temperature class	precipitation excess class	representative soil	representative crop	organic matter class
1	15-20	<250	loam	wheat	<3
2	10-15	<250	coarse sand	barley	<3
3	10-15	>250	coarse sand	maize/wheat	<3
4	10-15	<250	loam/sand	wheat	<3
5	5-10	<250	loam/sand	barley	<4
6	5-10	>250	loam♦	barley	<4
7	10-15	>250	clay	maize	<3
8	15-20	>250	clay	wheat	<2

♦: This scenario has a higher groundwater level due to the classification wet soils: 0.5 meters instead of 1.0 meters.

In the following table, a short topographical description of the regions is given:

Table A3.2. Definition of the European scenarios.

	Description
1	South West Spain; South Portugal
2	East Spain
3	North Portugal; North Spain; South France
4	Central France
5	North East France; Benelux; Germany; Denmark
6	Great Britain
7	North Italy: Corsica; North Greece
8	South Italy; Sardinia; Sicily; South Greece (Peloponessos); Crete

The organic matter content is a reference value for the upper 0.3 meters of the soil. For the calculation of leaching, this value is recalculated to obtain a value for the upper meter of the soil. The soil hydrological data were obtained from the Winand Staring series; They correspond with the horizons given in the following table:

Table A3.3. Horizons used to represent soil types.

soil type	Staring series horizon
loam	B15/O15
coarse sand	B1/O1♦
sand	B1/O1
loam/sand	B8/O9
clay	B10/O10

♦: Data on coarse sand were not reliable.

The boundary line between B and O horizons is situated at 0.5 m below soil surface. The scenario map was obtained from selection of areas visually. ARC/INFO 7.0.2., however, has an option with which the majority of grids can be determined within a certain area. For this, it is necessary to deliver the scenario map in a grid format and to overlay this grid map with a so called zonal grid. The function ZONALMAJORITY then calculates the majority of cells from the scenario grid for each zone in the zonal grid. The result depends on the choice of the zonal size.

Within scenarios 7 and 8, irrigation practices are commonly performed. Therefore, irrigation was applied by adding the amount of irrigation to the amount of precipitation. Since scenarios 1, 2 and 3 were derived from scenarios 7 and 8, it is assumed, that the irrigation practices are also performed within these areas. In Table A3.4 the irrigation regime used is given.

Table A3.4. Irrigation data for scenarios 1-3, 10 and 11.

day number	amount of irrigation (mm)
130	100
131	50
165	100
166	50
190	100
191	50
215	100
216	50

A3.2. Dutch scenarios

Due to the relatively small differences in precipitation (700-800 mm annually) and temperature (9-10 °C annually) within the Netherlands, the Dutch scenario map is not based on climate zones. Instead, determination of scenario regions is based on the Dutch soil map (1:250,000). Attributes in this map are amongst others soil codes (generalised version of the STIBOKA classification used in the soil map of the Netherlands scale 1:50,000) and organic matter content of the upper meter of the soil.

The soil map was further generalised into four main soil groups: sandy soils, loam soils, clay soils and peat soils. These groups were combined in ARC/INFO with three organic matter content classes: low (<3 %), moderate (3-6 %) and high (>6 %). Subsequently, the map containing these scenarios was combined with the municipality map of the Netherlands in order to perform a ZONALMAJORITY; in each municipality zone, the majority of a certain scenario is calculated. In this manner a scenario region map is obtained with 7 scenarios. In Table A3.5 the scenarios are defined. The map is shown in Chapter 3, Figure 3.9.

Table A3.5. Definition of Dutch scenarios.

scenario number	soil type	organic matter class	groundwater level	crop
1	sand	<3	1.0 m	maize
2	sand	3-6	0.8 m	beets
3	peat	>6	0.85 m	grains
4	loam	<3	1.0 m♦	maize
5	clay	<3	0.9 m	grains
6	clay	3-6	0.8 m	grains
7	clay	>6	0.9 m	potatoes

♦: No data were available, therefore the groundwater level was set at 1.0 meters.

The ZONALMAJORITY function was repeated to determine the groundwater level in each scenario region with the groundwater level classification map of the Netherlands as the thematic map and the scenario region map as the zonal map. Because of the fact that the crops chosen to calculate with in PESTRAS are not dominant forms of landuse in the Netherlands, determination of representative crops from the Dutch landuse map (LGN, 1986) was performed visually.

Like in the European scenarios, the soil types were represented in PESTRAS by the Winand Staring series. In Table A3.6, the corresponding horizon codes are given; the boundary line between the B and O horizons is situated at 0.5 meters below soil surface.

Table A3.6. Soil types and coding.

Soil type	horizon codes
sand	B1/O1
loam	B15/O15
clay	B10/O10
peat	O5♦

♦: Data on B horizons are not available.
The peat soils are represented by one horizon.

For the calculation of leaching, the combinations of Table A3.5 were input for PESTRAS, along with one (standard) meteorological input file. The figures enclosed visualise the meteorological conditions used in this exercise.

A3.3. German scenarios

The area of Germany was differentiated into 5 main soil types dependent on the depth and kind of development of the profile and the genesis of the soil type. For each of these soil types a typical profile was defined by deriving information from existing soil type data with those parameters the simulations with PELMO and PESTRAS require. Based on the Soil map of Germany a strong generalisation was necessary to confine to number of scenarios and to combine regions with a different soil structure into one soil scenario.

Table A3.7. Soil characteristics for the soils used for the German scenarios

Marshy Gleysol								
	Depth (cm)	pH (KCl)	OM (%)	OC (%)	Sand (%)	Silt (%)	Clay (%)	
Ap	0-25	6,4	3,3	1,90	20,0	60,0	20,0	
Go	25-70	6,5	1,8	1,05	22,0	61,0	17,0	
Gr	> 70	6,8	1,0	0,65	19,0	57,0	24,0	
Podsol								
	Depth (cm)	pH (KCl)	OM (%)	OC (%)	Sand (%)	Silt (%)	Clay (%)	Stones (%)
Ap	0-30	5,7	2,6	1,5	68,3	24,5	7,2	
Bhs	30-60	4,9	1,7	1,0	67,0	26,3	6,7	< 5
Bv	60-75	4,9	0,2	0,2	96,2	2,8	1,0	< 5
Cv	75-90	5,0	0,0	0,0	99,8	0,2	0,0	< 5
C	> 90	4,8	0,0	0,0	100,0	0,0	0,0	< 5
Luvisol								
	Depth (cm)	pH (KCl)	OM (%)	OC (%)	Sand (%)	Silt (%)	Clay (%)	
Ap	0-25	6,7	1,6	0,95	6,5	78,0	15,5	
Al	25-50	6,3	0,6	0,30	1,0	80,0	19,0	
Bt	50-80	6,3	0,4	0,20	0,5	72,0	26,5	
Cc	> 80	6,3	0,1	0,05	0,5	85,0	14,5	
Cambisol								
	Depth (cm)	pH (KCl)	OM (%)	OC (%)	Sand (%)	Silt (%)	Clay (%)	Stones (%)
Ap	0-25	6,4	3,3	1,90	21,0	58,0	21,0	< 10
Bv	25-40	5,6	1,8	1,05	18,0	61,0	21,0	< 40
Cv	40-60	6,0	1,0	0,65	24,0	57,0	19,0	< 80
Rendzina								
	Depth (cm)	pH (KCl)	OM (%)	OC (%)	Sand (%)	Silt (%)	Clay (%)	Stones (%)
Ap	0-20	7,4	3,7	2,15	22,0	58,0	20,0	< 40
Cv	20-30	7,6	2,7	1,55	27,0	56,0	17,0	< 80

Due to relatively big differences in precipitation (500 - 1.800 mm annually) and temperature (6 - 10 °C annually) in Germany, 9 climate scenarios have been differentiated. PELMO- and PESTRAS-simulations have been carried out with (daily) climatic data from the following climate stations. The different years represent a more or less typical year for the region what concerns precipitation and temperature.

Table A3. 8. Climate characteristics for the climate stations used for the German scenarios

Climate station	*Year*	*Precipitation*	*Average temperature*
Husum	1968	809 mm	8,4°C
Teterow	1986	552 mm	7,7°C
Hamburg	1978	778 mm	8,4°C
Berlin	1955	639 mm	8,9°C
Bad Kreuznach	1974	649 mm	10,4°C
Magdeburg	1980	483 mm	8,0°C
Schmallenberg	1968	1082 mm	6,0°C
Nürnberg	1985	664 mm	7,9°C
Oberstdorf	1956	1826 mm	6,2°C

The outcome of the combination of 5 soil scenarios with 9 climate scenarios were 13 soil-climate-scenarios for the area of Germany (See also chapter 3).

A3.4. Italian scenarios

Since data are not sufficient to define a more elaborate scenario map of Italy, this map was clipped from the European scenario map (the map is given in Chapter 3). Table A3. 9 shows the scenario data.

Table A3. 9. Italian scenarios.

scenario number	organic matter (%)	groundwater level (m)	representative crop	representative soil
1	1.24	2.0	maize	clay
2	1	no data (1.0)	wheat	clay

The soil types given in table A3.7. can be described with the Winand Staring Series of Stiboka (Table A3.3 and Table A3.5). With regard to the climatic classification, it can be stated, that the classification defined for the European scenarios are valid for the Italian scenarios, i.e. European scenarios 7 and 8 correspond to Italian scenarios 1 and 2, respectively. The input for PESTRAS with regard to the climatic data was also derived in the same manner as described in Section A3.1. This can also be stated with regard to irrigation data.

A4. Meta-information on spatial data

The following list of tables collects all meta information on the maps used in EUPHIDS. The tables are:

A4.1. Europe

Table A4. 1. Europe: landuse.

	Name layer: landuse
General	
Description	Landuse in EU
Spatial objects	Grid
Attributes	Land use features (numerical codes)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Good
Source	
Source material (map, digital)	Digital
Source organisation	RIVM
How is source information obtained ?	Available at RIVM for PANSOE project
Year	1993
Scale	1:1,000,000
Projection	Lambert azimuthal (Europe, not EC; centerpoint of projection differs)
Accuracy	Good
Operations	- altering projection - grid

Table A4. 2. Europe: organic matter.

	Name Layer: organic matter content
General	
Description	Reference organic matter content in the upper 0.3 metres of the soil in EU
Spatial objects	Grid
Attributes	Percentage organic matter
Scale	1:800,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	RIVM
How is source information obtained ?	Available for several projects within RIVM
Year	1993 (?)
Scale	1:800,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	None, grid was available

Table A4. 3. Europe: maximum rain in May.

	Name layer: Rainfall May
General	
Description	Maximum amount of rainfall per 24 in may in Europe
Spatial objects	Grid
Attributes	Rainfall data per 24 h. In may
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	Available at RIVM in geobase
Year	Variable, depending on weather stations (1950-1970)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Operations	- Joinitem on weather station point coverage with table with weather data for may per weather station - Interpolation on data (kriging); grid is result

Table A4. 4. Europe: maximum rain in October.

	Name layer: Rainfall October
General	
Description	Maximum amount of rainfall per 24 in October in EU
Spatial objects	Grid
Attributes	Rainfall data per 24 h. In October
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	Available at RIVM in geobase
Year	Variable, depending on weather stations (1950-1970)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Operations	-Joinitem on weather station point coverage with table with weather data for October per weather station
	- Interpolation on data (kriging); grid is result

Table A4. 5. Europe: sand/stone map.

	Name Layer: sand and stones.
General	
Description	Occurrence of sandy and/or stony soils in EU
Spatial objects	Grid
Attributes	Sand soil code
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE (based on FAO soil map of EC)
How is source information obtained ?	Available at RIVM in geobase
Year	On tape 1991
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	-Selecting sandy and/or stony soils and assigning an occurrence code to them -Grid

Table A4. 6. Europe: slope.

	Name layer: slope
General	
description	Slope classes in EU
spatial objects	GRID
attributes	Slope classes
scale	1:1,000,000
projection	Lambert azimuthal (EC)
accuracy	Unknown
Source	
source material (map, digital)	Digital
source organisation	CORINE (Based on analog FAO map)
how is source information obtained ?	Available at RIVM in GEOBASE
year	On tape 1991
scale	1:1,000,000
projection	Lambert azimuthal (EC)
accuracy	Unknown
Operations	Grid

Table A4. 7. Europe: meteo-scenario.

	Name Layer: meta scenarios for Europe
General	
Description	Scenario-areas for the EU based on meteo-data
Spatial objects	Grid
Attributes	Scenario number
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Moderate
Source	
Source material (map, digital)	Digital meteo map
Source organisation	RIVM (another project)
How is source information obtained ?	Available at RIVM
Year	1993
Scale	1:1,000,000
Projection	Lambert azimuthal (Europe, not EC: centerpoint of projection differs)
Accuracy	Good
Operations	-Select pnetto/temperature combinations and assign a scenario number to combinations -Aalter projection (Europe EC) -Generalisation of scenario-area (visual definition of areas) -Several minor adjustments to EC boundary maps -Grid

Table A4. 8. Europe: average temperature in May.

	Name Layer: Temperature in May
General	
Description	Average temperature in may in EUROPE
Spatial objects	Grid
Attributes	Temperature data in may
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	Available at RIVM in geobase
Year	Variable, depending on weather stations (1950-1970)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Operations	-Joinitem on weather station point coverage with table with weather data for may per weather station - interpolation on data (kriging); grid is result

Table A4. 9. Europe: Average temperature in October.

	Name layer: Temperature in October
General	
Description	Average temperature in October in EU
Spatial objects	Grid
Attributes	Temperature data in October
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	Available at RIVM in geobase
Year	Variable, depending on weather stations (1950-1970)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	High
Operations	- Joinitem on weather station point coverage with table with weather data for October per weather station - Interpolation on data (kriging); grid is result

A4.2. The Netherlands

Table A4. 10. The Netherlands: landuse.

	Name layer: Landuse
General	
Description	Land use in the Netherlands
Spatial objects	GRID
Attributes	Landuse features; numerical codes
Scale	1:250,000
Projection	Stereographic
Accuracy	High
Source	
Source material (map, digital)	Digital
Source organisation	RIVM
How is source information obtained ?	Available at RIVM in GEOBASE after purchase from SC-DLO
Year	1994
Scale	1:250,000
Projection	Stereographic
Accuracy	High
Operations	None (re-sizing of grids took place in XY)

Table A4. 11. The Netherlands: organic matter.

	Name layer: Organic matter
General	
description	Reference organic matter in the top 100 cm of the soil in the Netherlands
spatial objects	GRID
attributes	percentage organic matter
scale	1:250,000
projection	Stereographic
accuracy	Unknown
Source	
source material (map, digital)	Digital
source organisation	SC-DLO, RIVM
how is source information obtained ?	Available at RIVM, soil map of NL at 1:250,000 in GEOBASE
year	1994
scale	1:250,000
projection	Stereographic
accuracy	Unknown
Operations	GRID on organic matter content (value attribute)

Table A4. 12. The Netherlands: maximum rain in January.

	Name layer: Maximum rain in January
General	
Description	Maximum amount of rainfall per 24 hours in January
Spatial objects	GRID
Attributes	Rainfall data for January per 24 hours
Scale	1:250,000
Projection	Stereographic
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	Available at RIVM in GEOBASE
Year	Variable; dependent on weather station (1950-1970)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Netherlands from EU map of CORINE (alter projection) Linking rainfall data of CORINE to weather stations in the Netherlands Interpolating (Kriging); results in Grid

Table A4. 13. The Netherlands: sand/stone.

	Name layer: Sand/Stone
General	
description	Occurrence of sandy and/or stony soils in the Netherlands
spatial objects	GRID
attributes	Sand Soil Code
scale	1:250,000
projection	Stereographic
accuracy	Unknown
Source	
source material (map, Digital)	Digital
source organisation	SC-DLO (Netherlands)
how is source information obtained ?	Available at RIVM in GEOBASE
year	1991
scale	1:250,000
projection	Stereographic
accuracy	Unknown
Operations	Assigning numerical codes tot soil types (Command calculate) Selecting sandy/stony soils (command re-select followed by calculate) Grid

Table A4. 14. The Netherlands: slope.

	Name layer: slope
General	
description	Slope class map of the Netherlands
spatial objects	GRID
attributes	Slope classes
scale	1:250,000
projection	Stereographic
accuracy	Unknown
Source	
source material (map, Digital)	Digital (based on analog FAO map)
source organisation	CORINE
how is source information obtained ?	available at RIVM in GEOBASE in the soil map of EC (one of the attributes in the file)
year	On tape 1991
scale	1:1,000,100
projection	Lambert azimuthal (EC)
accuracy	Unknown
Operations	Clipping NL from EC slope map and alter projection GRID

Table A4. 15. The Netherlands: meteo-scenario.

	Name layer: meteo-scenario NL
General	
description	Soil/organic matter scenario map of the Netherlands
spatial objects	GRID
attributes	Scenario number
scale	1:250,000
projection	Stereographic
accuracy	Unknown
Source	
source material (map, digital)	Digital
source organisation	SC-DLO, RIVM
how is source information obtained?	Available as one coverage in GEOBASE at RIVM
year	1991
scale	1:250,000
projection	Stereographic
Operations	Generalisation of soil types into four main types Combination of these main types with organic matter classes; assignment of scenario numbers to combinations Grid on scenario number and zonalmajority with the nuts3 level of the Netherlands as the zonal grid

A4.3. Hupselse Beek (The Netherlands)

Table A4. 16. Hupselse Beek (The Netherlands): landuse.

	Name layer: Landuse
General	
Description	Land use in Hupselse Beek
Spatial objects	GRID
Attributes	Landuse features (numerical codes)
Scale	1:5000
Projection	Stereographic
Accuracy	Good
Source	
Source material (map, digital)	Map (analog), made by RIVM
Source organisation	RIVM
How is source information obtained ?	Obtained from another RIVM project (contact: G, van Eertwegh)
Year	1982
Scale	1:5,000
Projection	Stereographic
Accuracy	Good
Operations	Digitising from analog map boundaries of individual plots Assigning landuse code to each plot based on LGN-1 data Grid

Table A4. 17. Hupselse Beek (The Netherlands): organic matter.

	Name layer: Organic matter
General	
Description	Percentage organic matter in the upper metre of the soil in Hupselse Beek
Spatial objects	GRID
Attributes	Percentage organic matter
Scale	1:5,000
Projection	Stereographic
Accuracy	Good
Source	
Source material (map, digital)	Map (analog) made by STIBOKA
Source organisation	STIBOKA
How is source information obtained ?	Available at RIVM (contact: G, van Eertwegh)
Year	1982
Scale	1:5,000
Projection	Stereographic
Accuracy	Good
Operations	Digitising of the analog organic matter map Assigning values to the polygons obtained Grid

Table A4. 18. Hupselse Beek (The Netherlands): maximum rain in January.

	Name layer: Maximum rain in January
General	
Description	Maximum rainfall per 24 hours in Hupselse Beek
Spatial objects	GRID
Attributes	Rainfall data per 24 h.
Scale	1:5000
Projection	Stereographic
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	EC map of rainfall is available at RIVM in GEOBASE
Year	Variable, depending on weather stations (1950-1970)
Scale	1:1,000.000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Hupselse Beek from the weather station map (CORINE) and alter projection Assigning rainfall values to weather stations Interpolate (kriging); result is a grid

Table A4. 19 Hupselse Beek (The Netherlands): sand/stone.

	Name layer: Sand/Stone
General	
Description	Occurrence of sandy and/or stony soils in Hupselse Beek
Spatial objects	GRID
Attributes	sandy soils (numerical code)
Scale	1:5,000
Projection	Stereographic
Accuracy	Good
Source	
Source material (map, digital)	Map (analog) by STIBOKA
Source organisation	STIBOKA
How is source information obtained ?	Available at RIVM (contact: G, van Eertwegh)
Year	1982
Scale	1:5,000
Projection	Stereographic
Accuracy	Good
Operations	Digitising of the analog soil map Assigning soil codes to the polygons obtained Re-select sandy/stony soils and assign an occurrence code to them Grid

Table A4. 20. Hupselse Beek (The Netherlands): slope.

	Name layer: Slope
General	
Description	Slope (classes) in Hupselse Beek
Spatial objects	GRID
Attributes	Slope classes
Scale	1:5,000
Projection	Stereographic
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	EU-slope map is available at RIVM in GEOBASE
Year	Unknown
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Hupselse Beek from the EU Slope map and alter projection (Re-)defining slope classes Grid

A4.4. Germany

Table A4. 21. Germany: landuse.

	Name layer: Landuse
General	
Description	Landuse in Germany
Spatial objects	GRID
Attributes	Land use features (numerical codes)
Scale	1:250,000
Projection	UTM
Accuracy	Good
Source	
Source material (map, digital)	Digital
Source organisation	RIVM
How is source information obtained ?	Available at RIVM for PANSOE project
Year	1993
Scale	1:1,000,000
Projection	Lambert azimuthal (EUROPE, NOT EC; centerpoint of projection differs)
Accuracy	Good
Operations	Clipping Germany from EC landuse map Altering projection Grid

Table A4. 22. Germany: organic matter.

	Name layer: Organic Matter
General	
Description	Reference organic matter content in the upper metre of the soil in Germany
Spatial objects	GRID
Attributes	Percentage organic matter
Scale	1:250,000
Projection	UTM
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	RIVM
How is source information obtained ?	Available for several projects within RIVM
Year	1993 (?)
Scale	1:800,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Germany from Organic matter map; altering projection

Table A4. 23. Germany: maximum rain in May.

	Name layer: Maximum Rain in May.
General	
Description	Maximum amount of rainfall per 24 hours in May in Germany
Spatial objects	GRID
Attributes	amount of rainfall per 24 h.
Scale	1:250,000
Projection	UTM
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	available at RIVM in GEOBASE
Year	variable, depending on weather station (1950-1970)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	
	Clipping Germany from EC weather station map and assigning rain data to points in coverage; altering projection Interpolating (Kriging); result is a grid

Table A4. 24. Germany: sand/stone.

	Name layer: Sand/stone
General	
Description	Occurrence of sandy and/or stony soils in Germany
Spatial objects	GRID
Attributes	Sand soil code
Scale	1:250,000
Projection	UTM
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE (based on FAO soil map of EC)
How is source information obtained ?	Available at RIVM in GEOBASE
Year	On tape 1991
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Germany from the Soil map of the EC; altering projection Selecting sandy and/or stony soils and assigning an occurrence code to them Grid

Table A4. 25. Germany: slope.

	Name layer: Slope
General	
Description	Slope classes in Germany
Spatial objects	GRID
Attributes	Slope classes
Scale	1:250,000
Projection	UTM
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE (based on analog FAO map)
How is source information obtained ?	available at RIVM in GEOBASE
Year	On tape 1991
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Germany from slope map; altering projection Grid

Table A4. 26. Germany: meteo-scenario.

	Name layer: meteo-scenario for Germany
General	
General descriptions	Soil-climate scenarios for Germany
Spatial objects	Polygon
Attributes	Combination of 9 climate-scenarios and 5 soil-scenarios to 13 soil-climate scenarios
Scale	1 : 4.000.000
Projection	Conic projection (equidistant)
Accuracy	High
Source	
Source material	Map (for basis), scenarios developed by IUCT
Source organisation	Diercke-Weltatlas, 3rd edition (for basis)
How is source information obtained	
Year	1992
Scale	1:4.000.000
Projection	Conic-projections (equidistant)
Accuracy	High
Operations	Border line digitised, transformed into grids by RIVM

A4.5. Kreis Soest (Germany)

Table A4. 27. Kreis Soest (Germany): landuse.

	Name layer: Landuse
General	
General descriptions	Differentiation of 6 types of landuse
Spatial objects	Polygons
Attributes	Border lines between diverse types of landuse
Scale	1 : 50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Source	
Source material	Map
Source organisation	Landesvermessungsamt Nordrhein-Westfalen Muffendorfer Straße 19-21, 53177 Bonn
How is source information obtained	By terrestrial and aerial survey and observation
Year	1994
Scale	1:50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Operations	Polygons of landuse units digitised, transformed into grids by RIVM

Table A4. 28. Kreis Soest (Germany): organic matter.

	Name layer: Percentage of organic matter in soil
General	
General descriptions	Percentage of organic matter in soil (derived from soil map)
Spatial objects	Polygons
Attributes	% OM
Scale	1 : 50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Source	
Source material	Map
Source organisation	Geologisches Landesamt Nordrhein-Westfalen De Greiff-Straße 195, 47803 Krefeld
How is source information obtained	Laboratory measurements on representative sites, estimations by soil cartographers all over the area
Year	1986
Scale	1:50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Operations	Polygons of soil units digitised, transformed into grids by RIVM

Table A4. 29. Kreis Soest (Germany):maximum rain in January.

	Name layer: maximum rain in January
General	
General descriptions	Rainfall
Spatial objects	Polygon
Attributes	Rainfall
Scale	1 : 50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Source	
Source material	Map / Rainfall data from CORINE
Source organisation	Landesvermessungsamt Nordrhein-Westfalen Muffendorfer Straße 19-21, 53177 Bonn
How is source information obtained	Rainfall data from CORINE
Year	1931 - 1960 (average)
Scale	1:50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Operations	Border line digitised, transformed into grids by RIVM

Table A4. 30. Kreis Soest (Germany): sand/stone.

	Name layer: Percentage of sand/stone in soil
General	
General descriptions	Percentage of sand/stone in soil (derived from soil map)
Spatial objects	Polygons
Attributes	% sand/stone
Scale	1 : 50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Source	
Source material	Map
Source organisation	Geologisches Landesamt Nordrhein-Westfalen De Greiff-Straße 195, 47803 Krefeld
How is source information obtained	Laboratory measurements on representative sites, estimations by soil cartographers all over the area
Year	1986
Scale	1:50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Operations	Polygons of soil units digitised, transformed into grids by RIVM

Table A4. 31. Kreis Soest (Germany): slope.

Name layer: Slope	
General	
General descriptions	Slope
Spatial objects	Lines
Attributes	contour lines of altitude above sea level
Scale	1 : 50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Source	
Source material	Map
Source organisation	Landesvermessungsamt Nordrhein-Westfalen Muffendorfer Straße 19-21, 53177 Bonn
How is source information obtained	By terrestrial and aerial survey
Year	1994
Scale	1:50.000
Projection	Gauß-Krüger-Projection
Accuracy	High
Operations	Contour lines digitised, transformed into slope and grids by FUA/ESI

A4.6. Italy

Table A4. 32. Italy: landuse.

	Name layer: Landuse
General	
Description	Landuse in Italy
Spatial objects	GRID
Attributes	Land use features (numerical codes)
Scale	1:250,000
Projection	UTM
Accuracy	Good
Source	
Source material (map, digital)	Digital
Source organisation	RIVM
How is source information obtained ?	Available at RIVM for PANSOE project
Year	1993
Scale	1:1,000,000
Projection	Lambert azimuthal (EUROPE, NOT EC; centerpoint of projection differs)
Accuracy	Good
Operations	Clipping Italy from EC landuse map Altering projection Grid

Table A4. 33. Italy: organic matter.

	Name layer: Organic Matter
General	
Description	Reference organic matter content in the upper metre of the soil in Italy
Spatial objects	GRID
Attributes	Percentage organic matter
Scale	1:250,000
Projection	UTM
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	RIVM
How is source information obtained ?	Available for several projects within RIVM
Year	1993 (?)
Scale	1:800,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Italy from Organic matter map; altering projection

Table A4. 34. Italy: maximum rain in May.

	Name layer: Maximum Rain in a month
General	
Description	Maximum amount of rainfall per 24 hours in May in Italy
Spatial objects	GRID
Attributes	amount of rainfall per 24 h.
Scale	1:250,000
Projection	UTM
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE
How is source information obtained ?	available at RIVM in GEOBASE
Year	variable, depending on weather station (1950-1970)
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Italy from EC weather station map and assigning rain data to points in coverage; altering projection Interpolating (Kriging); result is a grid

Table A4. 35. Italy: sand/stone.

	Name layer: Sand/stone
General	
description	Occurrence of sandy and/or stony soils in Italy
spatial objects	GRID
attributes	Sand soil code
scale	1:250,000
projection	UTM
accuracy	Unknown
Source	
source material (map, digital)	Digital
source organisation	CORINE (based on FAO soil map of EC)
how is source information obtained ?	Available at RIVM in GEOBASE
year	On tape 1991
scale	1:1,000,000
projection	Lambert azimuthal (EC)
accuracy	Unknown
Operations	Clipping Italy from the Soil map of the EC; altering projection Selecting sandy and/or stony soils and assigning an occurrence code to them Grid

Table A4. 36. Italy: slope.

	Name layer: Slope
General	
Description	Slope classes in Italy
Spatial objects	GRID
Attributes	Slope classes
Scale	1:250,000
Projection	UTM
Accuracy	Unknown
Source	
Source material (map, digital)	Digital
Source organisation	CORINE (based on analog FAO map)
How is source information obtained ?	available at RIVM in GEOBASE
Year	On tape 1991
Scale	1:1,000,000
Projection	Lambert azimuthal (EC)
Accuracy	Unknown
Operations	Clipping Italy from slope map; altering projection Grid

Table A4. 37. Italy: meteo-scenario.

	Name layer: meteo-scenario Italy
General	
description	Climatic scenario map of Italy
spatial objects	GRID
attributes	Scenario number
scale	1:250,000
projection	Lambert Azimuthal (EC)
accuracy	Moderate
Source	
source material (map, digital)	Digital
source organisation	RIVM
how is source information obtained?	Available at RIVM
year	1993
scale	1:250,000
projection	Lambert Azimuthal (Europe, not EC; centerpoint of projection differs)
Operations	Clip from European climate scenario map (table A4.7., figure 3.6.) Recalculation of scenario numbers Grid

A4.7. Parco Sud (Italy)

Table A4. 38. Parco Sud (Italy): landuse.

	Name layer: Landuse
General	
Description	Landuse classes
Spatial objects	GRID
Attributes	Landuse classes
Scale	1:25.000
Projection	Universal Transverse Mercator (U.T.M.)
Accuracy	Moderate
Source	
Source material (map, digital)	Map
Source organisation	Parco Sud Board (PIM)
How is source information obtained ?	Land survey
Year	1990
Scale	1:25.000
Projection	U.T.M.
Accuracy	Moderate
Operations	Vectors (polygons of landuse) to grid (Arc/Info operation: POLYGRID)

Table A4. 39. Parco Sud (Italy): organic matter.

	Name layer: % OM
General	
Description	Percentage of OM per soil unit
Spatial objects	GRID
Attributes	% OM
Scale	1:50.000
Projection	Universal Transverse Mercator (U.T.M.)
Accuracy	Good
Source	
Source material (map, digital)	Map
Source organisation	Regional Board for Agriculture Development (ERSAL)
How is source information obtained ?	Measurements: 1 sample every 4 km^2
Year	1992
Scale	1:50.000
Projection	U.T.M.
Accuracy	Good
Operations	Vector (polygons of soil unit) to grid (Arc/Info operation: POLYGRID)

Table A4. 40. Parco Sud (Italy): maximum rain in November.

	Name layer: Rainfall
General	
Description	Amount of rain in November in mm
Spatial objects	GRID
Attributes	Amount of rain in November in mm
Scale	1:100.000
Projection	Universal Transverse Mercator (U.T.M.)
Accuracy	Moderate
Source	
Source material (map, digital)	Map
Source organisation	---
How is source information obtained ?	Census data
Year	Period 1960 - 1990
Scale	1:100.000
Projection	U.T.M.
Accuracy	Moderate
Operations	Vectors (polygons of amount of rain) to grid (Arc/Info operation: POLYGRID)

Table A4. 41. Parco Sud (Italy): sand/stone.

	Name layer: sand and stones
General	
Description	Presence of sand and stones in soil units
Spatial objects	GRID
Attributes	Sand and stones in soil units (yes/no)
Scale	1:50.000
Projection	Universal Transverse Mercator (U.T.M.)
Accuracy	Moderate
Source	
Source material (map, digital)	Map
Source organisation	Regional Board for Agriculture Development (ERSAL)
How is source information obtained ?	From soil survey
Year	1992
Scale	1:50.000
Projection	U.T.M.
Accuracy	Moderate
Operations	Vectors (polygons of soil unit aggregated) to grid (Arc/Info operation: POLYGRID)

Table A4. 42. Parco Sud (Italy): slope.

	Name layer: Slope
General	
Description	Slope classes
Spatial objects	GRID
Attributes	Slope classes
Scale	1:10.000
Projection	Universal Transverse Mercator (U.T.M.)
Accuracy	Good
Source	
Source material (map, digital)	Map
Source organisation	Lombardy region
How is source information obtained ?	From 1:10.000 maps of the Lombardy region
Year	1988
Scale	1:10.000
Projection	U.T.M.
Accuracy	Good
Operations	Vector (polygons of slope classes) to grid (Arc/Info operation: POLYGRID)

PART TWO: Future developments

A5. Qualitative assessment of run-off probability and intensity

The run-off algorithm currently implemented in the EUPHIDS program allows to quantify a PEC resulting from that process. However, since spatial information on parameters influencing run-off is not detailed enough or not available (e.g. slope, soil texture, water saturation of soil before a heavy rainfall, etc.) the calculation of Predicted Environmental Concentrations (PECs) for run-off might result in some kind of a *quantitative* „pseudo accuracy". In order to avoid such pseudo accuracy it should be considered to additionally implement a *qualitative* run-off assessment procedure in EUPHIDS which is based on a scoring system for the relevant parameters. The total score of spatial and substance inherent parameters serves as an indicator for the probability of occurrence and the intensity of run-off events.

As for the quantitative calculation of run-off, a distinction should be made between pesticide export in the water phase and export of pesticide adsorbed on soil particles. Both run-off pathways should be assessed individually. The highest score obtained by this procedures should then be further used and linked to the current EUPHIDS risk assessment structure. The qualitative assessment of run-off can be achieved as follows:

Run-off probability and intensity (water or sediment phase)

$$\approx \text{Slope x Rain x } \{(\text{Texture}_{\text{Soil}} \text{ x Koc}_{\text{Pest.}}) + (\text{Appl.-Techn. x Culture}) + (\text{Slopefact. x Rainfact.})\}$$

The occurrence of run-off is assumed to be basically dependent on the topography of the considered area (presence of slopes) and the probable occurrence of rain events sufficient to cause horizontal movement of water on the soil surface. Therefore, the exceedence of certain thresholds for these two parameters is used as trigger for the probability that run-off events might occur. Both parameters can either have a score of zero or of one (Table A5.1). The further parameters are connected to slope and rain in a multiplicative manner. By doing so, their scores count only in cases where either slopes are present or rain events are strong enough to cause run-off. They give additional information on the probable intensity of a run-off event. Closely interfering factors are connected multiplicatively to a group, groups are summed up to give the total score. Groups and individual parameters are not weighed equally but rated according to their relative importance for the intensity of a run-off event. Therefore, the group "Slope Factor x Rain Factor" can get the highest score (51 % of the maximum total score), "$\text{Texture}_{\text{Soil}}$ x Koc_{Pest}" has a max. weight of 31 %, and "Appl.-Techn. x Culture" is weighed least with 18 %.

A5.1. Parameters

The soil texture (Table A5.2) is an important parameter for the infiltration capacity of soils. Information on this parameter can be further used to draw assumptions on the stability of soil aggregates (particles released from unstable aggregates might limit the infiltration capacity by blocking soil pores) and the resistance of soil particles against transport by water (important to assess probable intensity of erosive processes). Soil texture data is attained from the CORINE soil map or from the soil scenarios which were established for the calculation of leaching.

The Koc (= Kom x 1.72) of a plant protection product is used to rate its expected sorption on soil particles (Table A5.3). Based on experimental evidence, the sorptive properties determine whether a pesticide is being transported preferentially in the water or sediment phase.

Application technique (Table A5.4) and culture (Table A5.5) might also influence the amount of pesticide lost due to run-off. The fixation in granules or seed coats and embedding in soil might attenuate pesticide loss compared with spraying the soil surface. Kind and state of culture determine the fraction of pesticide which might reach the soil as well as the erosive force of rain.

The slopefactor and the rainfactor (Tables A5.6 and A5.7) account for the steepness of slopes and the probable intensity of a rain event above the thresholds triggering run-off. Both parameters mainly influence the probable extend of particle erosion from agricultural areas since the erosive force of rain is determined by them.
The slope is read as slope class from the CORINE slope map (SLEC). The precipitation intensity is estimated for the month of pesticide application from the respective data for the climate scenarios used to calculate leaching. Rainfall intensity is provided as the maximum amount of rain within a day in the respective month. To avoid exaggeration of run-off risk by taking into account a unique rainfall event in the considered period of climate monitoring, 60 % of that value is taken as a realistic figure for precipitation intensity. Compared with the importance of slope and rain intensity for the pesticide export by the sediment phase of run-off the transport in the water phase is far less dependent on the steepness of the slope. Therefore run-off in the water phase and in the sediment phase are differently scored with respect to the parameter 'slope'. Rain intensity (amount per unit time) is also not that important for transport in the water phase as long as the amount of rainwater leaving the field is sufficient to dissolve all water soluble pesticide.

A5.2. Classification of Scores

Classification and description of scores is listed in Table 5.8. After a run-off event is rated as possible (score of "Slope" <u>and</u> "Rain" = 1), the minimum total score for run-off is 10.5. Already little exceedence of that minimum score should result in a shift from the low risk class to the medium risk class. The lower limit for the high risk class is set taking into account that the maximum score for the predominating run-off determining parameters "Slope Factor x Rain Factor" is 25. If this score has to be assigned, the risk should be considered as high irrespective whether the other two factor groups are scored minimally (min. score: "Slopefact. x Rainfact." = 1; "Appl.-Techn. x Culture" = 0.5).

A5.3. User Interface

The EUPHIDS user interface should allow to switch between quantitative and qualitative run-off assessment. In case of the qualitative assessment, the tables with the parameters should be displayed in order to tick the appropriate alternatives. The score calculations should be performed simultaneously for water phase and sediment phase. The run-off exposure route with the highest score should then be considered further and linked to the EUPHIDS risk assessment structure as described in the following paragraph.

A5.4. Use and Implementation of Results in current EUPHIDS Assessment Structure

The output of the score calculations could be displayed as run-off probability and severity maps. To give an indication of the risk posed by run-off on exposed ecosystems, probability and severity must be related to the inherent toxicity of the plant protection product and the background concentration expected to be already present as a result of spraydrift. This, in a pragmatic manner, can be achieved best by linking each run-off score class to a defined critical Predicted Environmental Concentration / (No-) Effect Level ratio (PEC/(N)EL) for the acute aquatic toxicity as proposed in Table A5.8. This procedure results in setting an additional safety factor based on probability and expected severity of a run-off event. The critical PEC/(N)EL ratios given in Table A5.8 yet need to be checked and may be changed by expert judgement.

Maps resulting from linking scores to critical PEC/(N)EL ratios could give an indication whether a pesticide can be used. For decision support, these maps can be further processed like PEC/(N)EL maps for spraydrift alone or the combination of spraydrift and quantitative run-off calculation.

Table A5.1: Slope and Rain.

SLOPE			
CORINE Slope Class	Slope [%]	Occurrence of Run-Off	Score
0	0	unlikely	0
a - d	4 - >30	probable	1
RAIN			
Calculation of Rain Intensity	Rain Intensity [mm /24 h]	Occurrence of Run-Off	Score
Maximum rainfall within 24 h in the month of pesticide application multiplied by the factor 0.6	≤ 15	unlikely	0
(to avoid exaggeration of run-off risk by taking the absolute maximum)	> 15	probable	1

Table A5. 2: Soil Texture.

Soil Texture	Soil properties	Characterisation	Run-Off Score water phase	Run-Off Score sediment phase
CORINE class 1:coarse Soil Scenarios: sand slightly loamy sand Histosols	<18 % clay >65 % sand 0 - 5 % clay >5 - 12 % clay	high infiltration capacity & coarse soil particles which cannot easily be moved by water additionally: high water capacity	1	1
CORINE class 2: medium CORINE class 3: medium fine Soil Scenarios: very loamy sand sandy loam slightly clayey loam	18 - 35 % clay and >15 % sand >35 % clay and <15 % sand 12 - 17 % clay >17 - 25 % clay >25 - 35 % clay	intermediate infiltration capacity, low cohesive forces between soil particles, therefore low aggregate stability and easy movement of (fine) soil particles	3	5
CORINE class 4: fine CORINE class 5: very fine Soil Scenarios: clayey loam loamy clay clay	>35 - 60 % clay >60 % clay >35 - 45 % clay >45 - 65 % clay >65 % clay	low infiltration capacity and high cohesive forces between very fine soil particles, therefore high aggregate stability and attenuated transport of soil particles by water	5	3

Table A5.3: K_{OC} of Plant Protection Product.

K_{OC}	Characterisation with respect to Run-Off	$\text{Run-Off}_{\text{Water Phase}}$ Score	$\text{Run-Off}_{\text{Sediment Phase}}$ Score
< 200	vertical movement into soil and export in water phase	2	1
200 - < 1000	export predominantly in water phase	3	2
> 1000	export predominantly in sediment phase	1	3

Table A5. 4: Application of Plant Protection Product.

Application as	Characterisation	Score
Seed Coating	Fixation in seed coat and embedding in soil attenuate export of pesticide by run-off	1
Granules	Fixation in granules and embedding in soil attenuate export of pesticide by run-off	1
Spray post emergence	A part of the pesticide is adsorbed onto the crop. Crop attenuates run-off	2
Spray pre emergence	Whole pesticide dose is deposited on top soil	3

Table A5.5: Culture.

Culture (Examples)	Characterisation of Cultures	Score Plant protection product used in an early developmental stage of the culture	Score PPP applied in a developmental stage where the plant canopy is developed to 50-100 %
Bare Soil	No protective plant cover	3	-
Potato Maize Beets Rape Sunflowers Legumes Hop Vine Orchards Tobacco	For a long time during the vegetation period soil is very sparsely covered by plants. Plant roots do not fix top soil very much. Soil is therefore insufficiently protected against erosive forces of rain	2.5	1.5
Wheat Barley Oat Rye Cereal-Leguminosae Fodder Mixes	Amount of plants, rooting pattern and plant canopy protect soils to some extend against erosive forces of rain	2.0	1.0
Pastures	Plant canopy and rooting pattern result in an effective protection of soil against erosive forces of rain	-	0.5

Table A5.6: Slope Factor

CORINE Slope Class	Mean Slope [%]	Score Run-Off$_{water\ phase}$	Score Run-Off$_{sedim.\ phase}$
a	4	3	3
ab	8	3	4
b	12	4	5
bc, c, cd, d	> 12	5	5

Table A5.7: Rain Factor

Intensity [mm /24 h] *	Score Run-Off$_{water\ phase}$	Score Run-Off$_{sedim.\ phase}$
> 15 - ≤ 25	3	3
> 25 - ≤ 40	4	4
> 40	5	5

* Maximum rainfall within 24 h in the month of pesticide application x 0.6

Table A5.8: Classification of Scores

Total Score	Classification
0	no risk: run-off needs not to be considered in the effects assessment
6 - 15	low risk: run off events may either occur seldom or may be not very intensive. The use of the assessed pesticide should be avoided unless the PEC/NEL ratio for the acute aquatic toxicity of spraydrift does not exceed 0.7. To achieve this, distance stipulations can be taken into consideration.
16 - 26	medium risk: run-off may occur and may be rather intensive. The use of the assessed pesticide should be avoided unless the PEC/NEL ratio for the acute aquatic toxicity of spraydrift does not exceed 0.5. To achieve this, distance stipulations can be taken into consideration.
> 26	high risk: the occurrence of run-off might be very probable or it might be very intensive. The use of the assessed pesticide should be avoided unless the PEC/NEL ratio for the acute aquatic toxicity of spraydrift does not exceed 0.1. To achieve this, distance stipulations can be taken into consideration.

A6. Multiple Applications

The present version of EUPHIDS only considers single applications. But there are a lot of pesticides which may be used several times within one season. Dependent on the time between two applications accumulation of pesticide concentrations in soil or surface water might be possible (see Figure A6.1).

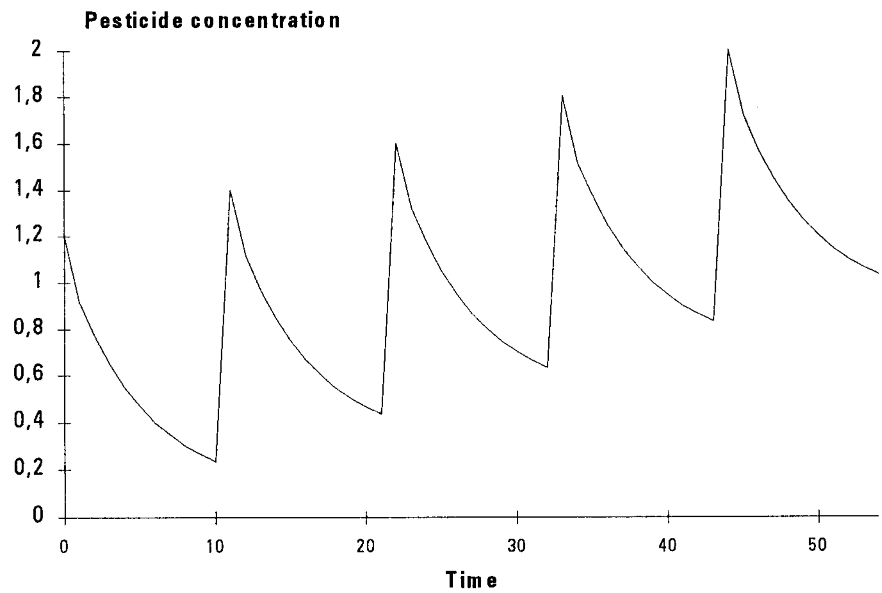

Figure A6.1: Pesticide concentration as a result of multiple applications.

Assuming constant time periods between following applications and constant pesticide input of all applications the resulting long term concentrations can be easily estimated.

$$c_0' = c_0 * \frac{\exp(K_T t_{app})}{\exp(K_T t_{app}) - 1} \qquad \text{(A6.1)}$$

t_{app}: time between two applications [d]
c_0': initial concentration for repeated applications at steady state
K_T: over all removal constant

This equation can be obtained by calculating the sum of all residues due to former drift or runoff events:

c(1): residue because of the latest application
c(2): residue because of the application before the latest application

$$c(1) = c_0 * \exp(-K_T * t_{app}) = c_0 * [\exp(-K_T * t_{app})]$$
$$c(2) = c_0 * \exp(-K_T * 2*t_{app}) = c_0 * [\exp(-K_T * t_{app})]^2$$
$$c(3) = c_0 * \exp(-K_T * 3*t_{app}) = c_0 * [\exp(-K_T * t_{app})]^3$$

...

$$c(n) = c_0 * \exp(-K_T * n*t_{app}) = c_0 * [\exp(-K_T * t_{app})]^n$$

$$\sum_{n=1}^{\infty} c(n) = c_0 * \sum_{n=1}^{\infty} [\exp(-K_T * t_{app})]^n$$

$$= c_0 * \sum_{n=1}^{\infty} 1 / [\exp(K_T * t_{app})]^n$$

$$= c_0 * \frac{1}{\exp(K_T * t_{app})] - 1} \qquad (A6.2)$$

If the current pesticide input is added to equation (2), equation (1) will be obtained. For calculating average concentrations in soil or in surface water it must be distinguished between two different situations:

A)The exposure time ($t_{exposure}$) is shorter than the time between two applications (t_{app}).

If the exposure time is shorter than the time between two applications the average concentrations will be calculated according to equation 3.1.1.13 or 3.1.2.5:

$$\bar{c} = \frac{c_0' * [1 - \exp(-K_T\ t_{exposure})]}{K_T * t_{exposure}} \qquad (A6.3)$$

Eq. (A6.3) can be easily transferred to eq (A6.4):

$$\bar{c} = \frac{c_0 * \exp(K_T\ t_{app}) [1 - \exp(-K_T\ t_{exposure})]}{[\exp(K_T\ t_{app}) - 1] * K_T * t_{exposure}} \qquad (A6.4)$$

where:

$\bar{c}$:	average concentration [mg/l]
c_0:	initial concentration [mg/l]
$t_{exposure}$:	The duration of the exposure [d]
t_{app}:	time between two applications [d].

B) The exposure time $t_{exposure}$ is longer than the time between two applications t_{app}. If the exposure is longer than the time between two applications the average concentration does not depend on the exposure time but only on t_{app} (the time between two applications). Therefore, $t_{exposure}$ has to be substituted by t_{app} in equation (A6.3) for calculating the average concentration.

$$\bar{c} = \frac{c_0' * [1 - \exp(-K_T\ t_{app})]}{K_T * t_{app}} \qquad (A6.5)$$

Equation (A6.5) can be simplified to eq. (A6.6.)

$$\bar{c} = \frac{c_0 * \exp(K_T t_{app}) * [1 - \exp(-K_T t_{app})]}{[\exp(K_T t_{app}) - 1] * K_T * t_{app}} \qquad (A6.6)$$

$$\bar{c} = \frac{c_0}{K_T * t_{app}} \qquad (A6.7)$$

A7. Estimation of PECs and pesticide risks for organisms of the terrestrial environment

According to the "Uniform Principles" (Council-Directive 94/43/EC) and many national pesticide risk assessment schemes pesticides must not adversely affect non target organisms (on the treated area) as well as species and functions of terrestrial ecosystems (adjacent to this area). To ensure this, the risk for certain species of concern has to be assessed during the admission procedure. Terrestrial species for which, according to the "Uniform Principles", data must be submitted are vertebrates and birds, honeybees and useful arthropods as well as earthworms and soil living bacteria. Therefore, the risk assessment procedure of EUPHIDS for terrestrial species and ecosystems needs to be based on these effect data. Since all that terrestrial species which have to be tested for the purpose of pesticide risk assessment must already, to a high extend, be protected from harm upon living on a treated field, it seems not very meaningful to consider terrestrial ecosystems as entities of their own in the risk assessment procedure as long as no further ecotox-tests with a broader and more representative spectrum of terrestrial organisms are available or more stringent safety margins for ecosystems are defined. It is therefore proposed to substitute the assessment of risk for terrestrial ecosystems by the assessment of risk for terrestrial organisms living on a treated field. To be able to calculate PEC/PNEC quotients as risk estimates, appropriate field-scenarios for the calculation of PECs have to be established. According to the Uniform Principles the following criteria and risk quotients need to be kept:

Organisms	Criteria and Risk Quotients
Soil micro-organisms:	≤ 25% C- or N-mineralization loss after 100 days in lab studies
Honeybees:	$LD50_{oral, contact}$ [µg/bee] / $Dose_{maximum}$ [g/ha] ≥ 50
Useful arthropods:	< 30% mortality at maximum intended application dose
Earthworms:	short term LD50 / PEC ≥ 10 ≈ PEC /LD50 ≤ 0.1
	long term NOEC/PEC ≥ 5 ≈ PEC /NOEC ≤ 0.2
Birds and vertebrates:	short term LD50 / PEC ≥ 10 ≈ PEC /LD50 ≤ 0.1
	long term NOEC/PEC ≥ 5 ≈ PEC /NOEC ≤ 0.2

The respective toxicity test results (LD50, NOEC, etc.) can be stored in the EUPHIDS pesticide database and retrieved from there. The first three groups of organisms only need to be checked for compliance with the standards set by the Uniform Principles (Yes/No answer in case of bacteria; simple calculation $LD_{50}/Dose_{maximum}$ in case of honeybees; check that intended dose does not cause more than 30% mortality of beneficial arthropods). Results for these groups do not rely on spatial variables. Therefore, the implementation of these groups in the EUPHIDS functionality for the terrestrial risk assessment seems not to be of high priority. But earthworm, bird and vertebrate exposure scenarios must be established and included in the EUPHIDS terrestrial risk assessment routine in order to be able to calculate the exposure (PEC) for these groups of animals.

A7.1. Selection of Relevant Exposure Pathways and Exposure Scenarios

Terrestrial organisms living on a field might be exposed to pesticides through different exposure pathways. Plants and non vertebrate animals are exposed by direct spraying, soil organisms like earthworms and also plant roots via the soil solution. Birds and vertebrates might be more indirectly threatened by ingestion of contaminated food.
The scenario approach should comprise important processes governing the exposure and environmental concentration of a pesticide, e.g. the mode of application (spray, granules etc.), interception by crop and soil, biomass (growth stage) of the crop and processes like volatilisation from plant surfaces and uptake by roots, further the penetration depth into soil (in EUPHIDS assumed to be 0.05 m during short term exposure and 0.2 m during long term exposure). Since the pesticide concentration in plants and soil is dependent on standing crop and culture specific interception factors, for many crops and growth stages (application dates) figures for biomass and interception rates must be gathered in a database (Table A7.1). Where appropriate, interception percentages can be taken from USES (1994).

Table A7.1. a) Biomass and Interception factors (spray application) for different crops and soil. (The table is thought as an example to explain the approach and needs to be extended by further data)

	Application early, after emergence			Application late, fully in leaf		
	Biomass[#] above ground [kg/ha]	Interception* Plant	Interception* Soil	Biomass[#] above ground [kg/ha]	Interception* Plant	Interception* Soil
Default	1 000	0.10	0.80	40 000	0.70	0.20
Bare Soil (pre emergence)	0	0.00	0.90	-	-	-
Crops						
Wheat (Cereals)	2 500	0.10	0.80	60 000	0.80	0.10
Rape	1 500	0.10	0.80	45 000	0.80	0.10
Maize	...	...	...	...	...	...
Sugarbeets	...	...	...	...	...	...
Tomato	...	...	...	...	...	...
Wine	...	...	...	...	...	...
Orchards	...	0.40	0.50	...	0.70	0.20

figures for wheat and rape taken from Fischbeck (1982)

* figures for interception taken from USES (1994)

Table A7.1 b) Interception factors and exposure routes to be considered for non-spray application modes

Mode of application	Scenario: Biomass [kg/ha]	Partition: Plant	Partition: Soil	Comments
Granules	--	0.0	1.0	Calculation of PEC_{soil} only. PEC/NEC estimates for soil living organisms (bacteria, worms) and probably worm eating animals.
Treated Seeds	Usual amount of seeds for the different crops	0.3	0.7	PEC/NEC estimates for seed eating birds and soil living organisms (bacteria, worms) and probably worm eating animals.
Directly into Soil	--	0.0	1.0	Calculation of PEC_{soil} only. PEC/NEC estimates for soil living organisms (bacteria, worms) and probably worm eating animals.

A7.2. PEC Estimation for Treated Fields

As a first step, only spraydrift applications (Table A7.1) are considered for the calculation of Predicted Environmental Concentrations (PEC). The functionality to calculate the PECs for other application techniques like seed dressing and granules may be added later. PEC estimation for treated fields is performed for soil and plant material. It takes account for processes like abiotic and biotic degradation in soil (DT_{50} of pesticide), evaporation from plant surfaces, percentage of spraydrift interception by plants and deposition on soil, and pesticide uptake from soil by plants, which might alter and in many cases diminish predicted pesticide concentrations for plants and soil. As a rough estimation it is assumed that pesticide spray is deposited evenly on all plant surfaces and that deposits on the soil are homogeneously distributed in the first 5 (short term) or 20 cm (long term) of top soil. Output of the PEC calculations should be the initial concentrations (PIEC = short term PEC) and a time averaged PEC over the considered time interval (long term PEC). The time interval should be related to the duration of the toxicity test or should be a default of 7, 28, 50 or 100 days (according to Council-Directive 95/36/EC which is an amendment to Directive 91/414/EC).

A7.3. Exposure of Plants

The percentage of spraydrift-deposition of a pesticide is dependent on the treated crop and its developmental state (apart from spraying equipment and weather conditions). It can be expressed as % of the applied dose or as [kg a.i./ha] respectively [mg a.i./m^2].

A7.3.1.Short Term PEC for Plants

The short term PEC of the aboveground plant material is the predicted initial concentration (PIEC) and assessed using the equation:

$$PEC_{pl}.st\ [mg/kg] = PIEC_{pl} = A_D\ [mg/m^2] * F_i,plant * FG^{-1}\ [kg/m^2] \quad (A7.1)$$

in which:

$PEC_{pl}.st$ = concentration of the pesticide in/on the plant material [mg a.i./kg plant]

A_D = applied dose on target area [mg/m^2] (= A_D [kg/ha] * 100)
FG = fresh weight of aboveground phytomass [kg/m^2] (this figure is retrieved from a table with phytomass data on specific cultures and application dates. See Table A7.1)
F_i,plant = portion of pesticide intercepted by the crop (100% = 1, see Table A7.1)

A7.3.2. Long Term PEC for Plants

The long term PEC of the aboveground plant material is calculated taking into account the percentage of intercepted pesticide, volatilisation from plant surface, and uptake via root.

$$PEC_{pl}.lt\ [mg/kg] = (PIEC_{pl} * (1 - e^{-(Volat * t)}) / (Volat * t) + C_{urt} \qquad (A7.2)$$

in which:

$PIEC_{pl}$ = Initial conc. on plants due to spraydrift (= PEC_{pl}.short term = A_D*F_i*FG^{-1})
t = time in seconds (86400 s = 1d)
Volat = Time dependent volatilisation of a.i from plant surface. Volatilisation can be calculated if substance specific properties like vapour pressure and molecular weight are known (Emans et al., 1992). Compound concentration in spray solution and air temperature (spatial variables) are also required.

$$Volat\ [mg/m^2 * s] = (3 * PIEC_{p.sd}\ [mg/m^2] * E_d\ [mg/m^2 * s]) * (2 * R_o\ [m] * C_o\ [mg/m^3])^{-1} \qquad (A7.3)$$

in which:

R_o = droplet radius: 0.2 * 10^{-3} m (constant)
C_o = conc. of a.i. in spray solution [mg/m^3]
E_d = evaporation density [mg/m^2 * s]: (D * V_p / R * T * Lt) * M *10^6
R = gas constant: 8300 J/kmol * K(elvin)
T = temperature: 293 K (or spatially variable according to climate map)
Lt = laminar thickness of leaf boundary layer: 0.03 * 10^{-3} mm (constant)
V_p = vapour pressure (Pa) of a.i.
D = diffusion coefficient: 8.8 * 10^{-9} * (R * T / M)$^{2/3}$
M = molecular weight [kg/kmol]
C_{urt} = Conc. in plants due to uptake by roots from soil solution: It can be calculated if the pesticide concentration in the soil solution (see estimation of PEC_{soil}), soil bulk density and water content (spatial variable) and the Kow of the pesticide are known. With this information a bioconcentration factor from transportation stream solution in a plant to concentration in stem tissue is calculated as follows (Emans et al., 1992):

$$C_{urt}\ (mg/kg) = SCF * TSCF * C_{soil.sln} \qquad (A7.4)$$

in which:

SCF = Stem Concentration Factor ($0.82 + 10^{0.95 * \log Kow - 2.05}$)

TSCF = Transportation Stream Conc. Factor (0.748 * $e^{-(\log Kow - 1.78)2/2.44}$
$C_{soil.sln}$ = Concentration of a.i. in soil solution (mg/kg) (see Section A7.4)

The long and short term PECs for plants resulting from the above calculations should be used for assessing risk for herbivores. The doses for these organisms can be calculated if their daily food ingestion is known.

A7.4. Exposure of Soil

PEC_{soil} is principally calculated as already explained in Chapter 3. The formula needs to be extended by a variable accounting for crop and application time dependent interception factors as given in Table A7.1.

A7.4.1.Short Term PEC Soil

$$PEC_{soil}.st = PIEC_{soil.sd} = A_D \; * \; F_i,soil \; * \; W_{soil}^{-1} \qquad \text{(A7.5)}$$

in which:
$PIEC_{soil.sd}$ = Initial PEC_{soil} via spraydrift
A_D = applied dose on target area [mg/m^2] (= A_D [kg/ha] * 100)
F_i,soil = portion of pesticide intercepted by soil (100% = 1, see Table A7.1)
W_{soil} = weight of affected soil in kg/m^2 = D_{soil} [m] * BD_{soil} [kg/l] * 1000,
D_{soil} = penetration depth of a.i. [0.05 m],
BD_{soil} = bulk density soil (default 1.5 kg/l or map input).

A7.4.2.Long Term PEC Soil

The long term PEC_{soil} is calculated as average concentration over a prolonged period of time (7, 28, 50, 100 days or according to the relevant ecotox test). Degradation of the pesticide is considered.

$$PEC_{soil}.lt = PIEC_{soil.sd} * (1 - e^{-(ks * t_{exposure})}) / k_s * t_{exposure} \; * \; K \qquad \text{(A7.6)}$$

in which:
$PIEC_{soil.sd}$ = initial PEC_{soil} via spraydrift (according to section 4.1, short term PEC. Except of the penetration depth of the pesticide, which is 0.2m)
$t_{exposure}$ = Interval of exposure (duration of considered single species test or default)
k_s = removal $konstant_{substance}$ = ln2/DT_{50} [d^{-1}]
K = correction term for soil temperature

A7.4.3.Partition of Pesticide between Soil Particles and Soil Solution

This parameter is needed for the calculation of pesticide uptake by plant roots. Under consideration of the K_d-value of the substance the distribution between and the concentration in the solid phase and pore water of soil can be calculated. For the calculation of the K_d-value from the K_{OC}-value the soil organic carbon content needs to be known (map input).

$$C_{soil.par} \text{ [mg/kg]} = K_d * C_{soil.sln} \text{ [mg/l]} \qquad \text{(A7.7)}$$

in which:

$$K_d = \frac{K_{OC} \; * \; C_{org}\,(\%)}{100\,(\%)}$$

C_{org} = organic carbon content in soil (spatial variable taken from maps)
K_{OC} = K_{OM} * 1.72 (transformation factor if K_{OC} data is not available)
$C_{soil.par}$ = Fraction of a.i. adsorbed by particles
$C_{soil.sln}$ = Fraction of a.i. dissolved in soil water

$$C_{soil.sln}\,[mg/l] = C_{soil.total}\,[mg/kg] * (Kd + F_{sw}/D_b\,[kg/l])^{-1} \qquad (A7.8)$$

in which:
$C_{soil.total}$ = $C_{soil.par} + C_{soil.sln}$
F_{sw} = Fraction of soil water (vol/vol). This parameter is variable depending on space and time. Unless specific information is available the default water content of 1 l soil is 0.3 l.
D_b = Soil bulk density soil (default 1.5 kg/l or taken from standard scenarios for leaching)

A7.5. Relating PECs to Toxicity Test Results for Estimating Risk

Short and long term PECs of soils and plants calculated as described above are compared with the (No-) Effect Levels (N)ELs for earthworms as well as herbivorous birds and mammals in order to get the appropriate risk quotients. (N)ELs can be obtained by the different evaluation and extrapolation methods included in EUPHIDS (e.g., Uniform Principles, EPA, Aldenberg & Slob etc.). Also for birds and mammals feeding on earthworms or insects scenarios are given which allow to calculate risk for such animals.

In case of earthworms, the LC_{50} or NOEC data can directly be related to the short or long term PECs for soil. For birds and mammals pesticide doses need to be calculated under consideration of PEC_{plant} and PEC_{soil}, amount of food ingestion and body weight. These doses then are related to the respective LD_{50}s, NOELs or NOAELs in order to calculate the risk quotients. Body weights and food ingestion rates for birds and mammals of various sizes are given in Table A7.2. Dependent on lacking data and to facilitate calculations, it is assumed that all plant material ingested by herbivorous animals, irrespective whether it is leaves, seeds, pods, fruits etc., is contaminated with the concentration estimated by the PEC_{plant} calculation and that it has the same surface to mass ratio and caloric energy and water content, so that different plant diets (e.g. whether an animal is feeding on leaves or seeds) do not influence the dose calculated to be ingested by the animal.

I. The risk quotient for herbivorous animals is then calculated as follows:

1. Calculation of the actual oral dose (relevant PEC):

a) short term (A7.9)

$Dose_{oral}st]$ =

$PEC_{plant}st$ [mg a.i. / kg plant] * Specific Daily Food Intake of animal X [kg / kg BW]

b) long term (A710)

$Dose_{oral}lt$ [mg a.i. / kg BW * d] =

$PEC_{plant}lt$ [mg a.i. /kg plant]*Specific Daily Food Int.of animal X [kg / kg BW * d] * F_{FR}

F_{FR} = factor food resources: it is assumed that only a certain percentage of daily food is taken from the treated area. The default is 70 % (F_{FR} = 0.7)

2. Calculation of the risk quotient:

(A7.11)

$$RQ = \frac{Dose_{oral}st, lt \text{ [mg a.i. / kg BW (* d)]}}{\text{(No-)Effect Level } (LD_{50}, \text{NOEC, NO(A)EL etc) [mg a.i. / kg BW (* d)]}}$$

Example 1:

LD_{50} Rabbit = 220 mg/kg BW; $PEC_{plant}st$ = 7 mg/kg

$Dose_{oral}st$ = 7 [mg a.i. / kg] * 0.408 [kg food / kg BW] = 2.86 [mg a.i. / kg BW]

RQ = $Dose_{oral}st$ (2.86 [mg / kg BW]) / LD50 (220 [mg / kg BW]) = 0.013

Example 2:

NOEL Mouse = 11.3 mg/kg BW x d; $PEC_{plant}lt$ = 3.3 mg/kg

$Dose_{oral}lt$ = 3.3 [mg a.i. / kg] * 0.852 [kg food / kg BW * d] * 0.7 (F_{FR})
= 1.97 [mg a.i. / kg BW * d]

RQ = $Dose_{oral}lt$ (1.97 [mg / kg BW *d]) / [NOEL (11.3 [mg / kg BW * d])
= 0.174

Table A7.2: Scenario data on mammals and birds

Species	Feeding Type (4)	Body Weight kg (BW)	Percentage vegetable / animal foodstuffs	Food Uptake kg (dw) / d (dry weight) (5)	Food Uptake kg (ww) / d (wet weight) (6)	Specific Food Uptake kg (ww) / kg (BW)
Rabbit[1]	h	1.9	100/0	0.1164	0.776	0.408
Mouse[1]	h	0.027	100/0	0.0035	0.023	0.852
Shrew[2]	i, w	0.012	0/100	0.0018	0.012	1.000
Rat[1]	h	0.370	100/0	0.0303	0.202	0.546
Finch[3]	h	0.018	100/0	0.0046	0.031	1.722
Tit[3]	i	0.018	0/100	0.0046	0.015	0.833
Blackbird[3]	w, i	0.118	0/100	0.0230	0.077	0.653
Quail (Bobwhite)[3]	h	0.170	100/0	0.0143	0.095	0.559
Phesant[3], domestic Fowl	h	1.200	70/30	0.0619	0.351	0.293

[1] according to USES (1994), [2] acc. to Brohmer (19982), [3] acc. to Kenaga (1973)

(4) h = herbivore, i = insectivore, w= earthworms

(5) Calculated acc. to USES module Daily Food Intake, p. 101

(6) Estimates based on water contents of 85% for plants and 70% for animals

II. For <u>animals feeding on earthworms or insects</u> the calculation of the relevant PECs is more complicated:

For worm eaters like blackbirds a pesticide concentration in earthworms may be estimated as:

PEC_{worm}, st, lt = BCF_{worm} x PEC_{soil}, st, lt

where PEC_{soil}, st, lt is calculated as described above (PIEC for short term exposure and time averaged concentration for X days depending on the duration of the toxicity test for long term exposure). If an experimentally derived bioconcentration factor (BCF) for earthworms is not available in the pesticide dossier, it can be calculated as follows (USES, 1994, page 92):

$$BCF_{worm} = \frac{K_{worm\text{-}porewater} * D_b,soil}{K_{soil\text{-}water} * D_b,worm} \quad (A7.12)$$

in with:

$K_{worm\text{-}porewater}$ = 0.25 * Kow (Kow = octanol-water partition coefficient of the pesticide)
$K_{soil\text{-}water}$ = soil-water partition coefficient (default: 0.3 l water/ 1.0 l wet soil)
D_b,soil = bulk densitiy soil (default 1.5 kg/l or taken from standard scenarios for leaching)
D_b,worm = bulk density worm: 1.05 kg/l

An actual oral dose (relevant PEC) for blackbirds and other worm eating animals can be obtained from PEC_{worm},st,lt as described for herbivores from PEC_{plant}. As for long term risk assessment of herbivores, it is assumed that no more than 70% of the worm prey is taken from the treated area.

III. For <u>animals feeding on small insects</u> a PEC for this insect prey is calculated according to the following scenario:
It is assumed that 50 % of the body surface is hit by pesticide spray. The dose deposited on these 50% of body surface is estimated to amount to a certain percentage of the nominal dose calculated as deposition on an equally large area of the treated field. This percentage differs since soil surface together with the plant surface sum up to a total surface area usually exceeding the sole soil surface several times (Table A7.3).

Table A7.3: Pesticide doses on insects in dependence of mode of application and type of culture

Scenario	Interception factor for insect prey (F_i,ins) % of nominal dose [mg/m^2] on insect body surface
Spray on soil (pre emergence)	100
Spray post emergence	70
Spray culture fully in leaf	50
Granules	-
Seed dressing	-
Application into soil	-

The body surface of insects is calculated assuming cylinders of a certain length and diameter (Table A7.4). With such data and the information given in table 3 it is possible to calculate the surface contamination of insects. Body burdens can be calculated by means of relating the surface dose to the body weight.

Table A7.4: Scenario data on insects

Insect	body length (h) [m]	body radius (r) [m]	50% of body surface[1] [m^2]	body weight[2] [kg]
small beetle, fly	1.0 E-2	0.20 E-2	0.754 E-4	0.1319 E-3
caterpillar	3.5 E-2	0.25 E-2	2.945 E-4	0.7216 E-3

1 body surface = 50% of a cylinder surface = 0.5 * $((2\pi r * h) + (2 * \pi r^2))$

2 body weight = volume of a cylinder (πr^2 * h) [m3] * specific density [≅ 1050 kg/m^3]

Calculation of body burdens and PEC_{prey}:

(A7.13)

$$\text{Body burden } B_b \text{ [mg a.i.]} = A_D \text{ [mg a.i. / m}^2] * S_B [m^2] * F_i\text{,ins}$$

in with:

A_D = applied dose on target area [mg/m^2] (= A_D [kg/ha] * 100)

S_B = 50% of body surface [m^2] (table 4)

F_i,ins = interception factor for insect prey depending on crop, crop growth stage and application technique (table 3)

$$PEC_{insect} \text{ [mg a.i. / kg prey]} = \frac{\text{Body burden [mg a.i]}}{\text{Body weight [kg]}} \quad \text{(A7.14)}$$

For the food intake scenario of insectivorous animals it is assumed that the insect prey consists of 50% beetles/flies and 50% caterpillars:

$$PEC_{prey} \text{ [mg/kg]} = (PEC_{beetle/fly} + PEC_{caterpillar}) / 2 \quad \text{(A7.15)}$$

With this initial PEC for insect prey and the specific food intake of the insectivores actual doses (relevant PECs) for short term exposure can be calculated in the same way as already described for herbivores. Because of many uncertainties (death rate and mobility of insects, population turnover, degradation/metabolisation on/in insects etc.) it seems not meaningful to attempt calculation of long term PECs in a similar manner.

(A7.16)

$Dose_{oral}$st [mg a.i. / kg BW] =

PEC_{prey}st [mg a.i. / kg] * Specific Daily Food Intake of insectiv. animal [kg / kg BW]

(A7.17)

$$RQ\text{, st} = \frac{\text{(No-) Effect Level (}LD_{50}\text{, NOEC, NO(A)EL etc) [mg a.i. / kg BW (* d)]}}{Dose_{oral}\text{st, lt [mg a.i. / kg BW (* d)]}}$$

A7.6. Features of the User Interface for Terrestrial Risk Assessment

The user should be asked to select crop and crop growth stage (time of application) from a table (cf. Table A7.1). The growth stage also governs the pesticide body burden of insects (amount of pesticide intercepted by prey, Table A7.3) so that data of these tables may be linked. Further, the risk assessor should be able to choose a herbivorous, insectivorous and worm eating bird and mammal species from a table (cf. Table A7.2). Since that choice results in 6 dose calculations for long and short term risk estimations each, it could be useful to implement a functionality that automatically selects the most sensitive feeding type (herbivorous, insectivorous, worm) after the calculation of the risk quotients so that only the results for that particular bird and mammal are displayed and visualised as maps.

A8. Alternative description of runoff decay

Runoff of pesticides into aquatic ecosystems is calculated in EUPHIDS by an empirically derived set of equations (see Section 3.) that may or may not consider the decay of pesticide concentrations in runoff depending on the distance of surface waters from the area of application. This empirical approach assumes equilibrium between water and suspended solids. The runoff system is treated as a black box, i.e. the processes are not considered. In this chapter an alternative approach to runoff decay is described. This theoretical approach describes the processes within the runoff system dynamically on the basis of mass balances for the media (i.e. water and sediment) and a compound. Since it is not the purpose of this chapter to deliver a complete model, only a brief overview of the processes and a description of the differential equations is given.

A8.1. Process visualization.

In figures A8.1 and A8.2, a visualization of the processes considered is given for a certain part of the runoff system (control volume). The runoff event is assumed to consist of several transport processes. These processes are:

Precipitation. Precipitation is assumed to be the driving force behind the water flow and the suspension of particles. Evapotranspiration is not taken into account.

Suspension of solid particles. It is assumed, that suspension of particles is caused by the impact of precipitation and the transfer of kinetic energy of the raindrops to potential energy of the solid particles. Compounds are asssumed to be introduced into the runoff system in this manner.

Transport of dissolved compounds (water flow, infiltration) and compounds sorbed onto the suspended solids. Horizontal transport takes place if:

- ♦ The slope is larger than zero;
- ♦ The infiltration capacity is lower than the precipitation intensity;
- ♦ Ponding of water on the soil surface exceeds a maximum value.

The water flow is assumed to be laminar.

Sedimentation of suspended solids. Sedimentation is assumed to occur due to gravity only.

Chemical interaction between water and solids. It is assumed, that the sorption interaction between water and suspended solids and water and settled solids can be described with first order kinetics. Other chemical phenomena, like transformation of a compound are assumed not to occur.

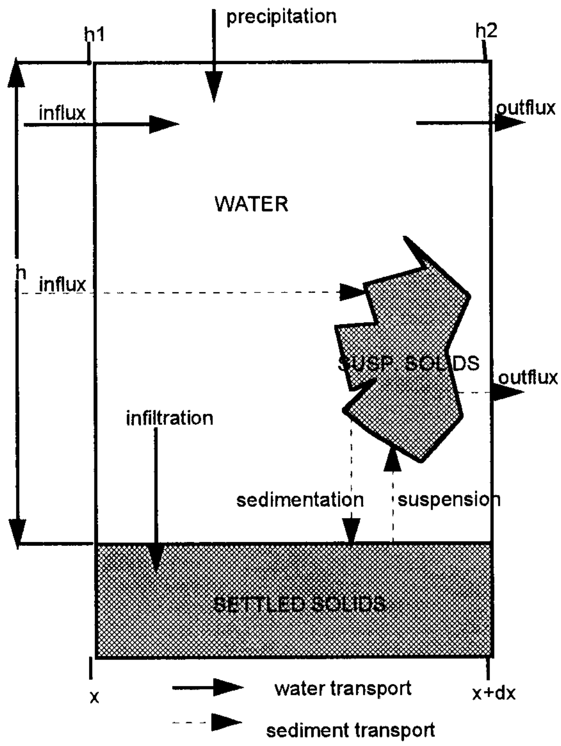

Figure A8.1. Fate of media within a control volume part of the runoff system.

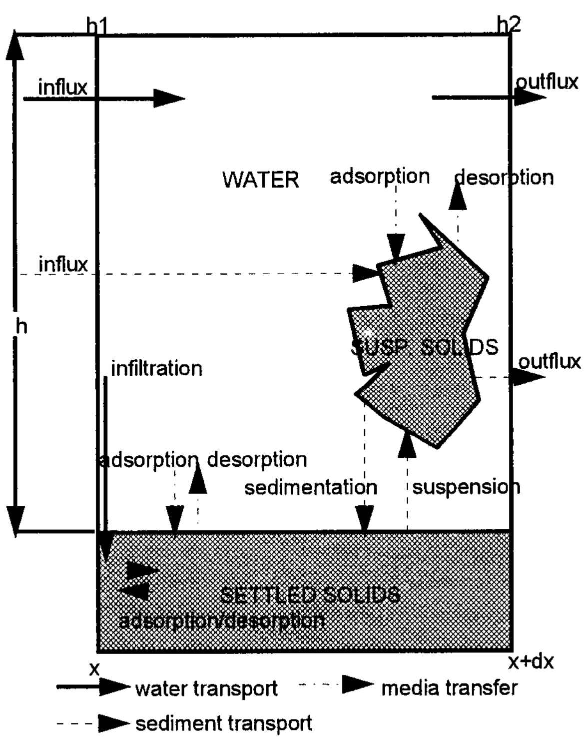

Figure A8.2. Fate of compounds within a control volume part of the runoff system.

A8.2. Mathematical description

Media

Water

For water, the following differential equation can be derived (Bird et al., 1960):

$$\frac{\partial h}{\partial t} = -\frac{\partial (q_r h)}{\partial x} + R - I \quad \text{(A8.1)}$$

q_r and h, average fluid velocity and height of the water column, respectively are related using the Manning equation (assuming laminar flow) (Morgan, 1986):

$$q_r = \frac{h^{1.7}(\tan\theta)^{0.95}}{n} \quad \text{(A8.2)}$$

For R, the daily amount of rainfall, tables can be used. I, the infiltration rate, is described with the following empirical function (Morgan, 1986):

$$I = K_{sat} + A(t^{-0.5}) \quad \text{(A8.3)}$$

Suspended solids

For suspended solids, the following differential equation can be derived (Bird et al., 1960):

$$\frac{\partial X_s}{\partial t} = -\frac{\partial F_s}{\partial x} + \left[X_{ds} - \frac{\overline{V}\sin\alpha_z}{h} X_s \right] \quad \text{(A8.4)}$$

F_s, the sediment flux, is assumed to consist of a convective part and a dispersive part (van Mazijk, 1983):

$$F_s = q_r X_s - D_s \frac{\partial X_s}{\partial x} \quad \text{(A8.5)}$$

Substitution in equation A8.4 gives:

$$\frac{\partial X_s}{\partial t} = -\frac{\partial (q_r X_s)}{\partial x} + D_s \frac{\partial^2 X_s}{\partial x^2} + \left[X_{ds} \frac{\overline{V}\sin\alpha_z}{h} X_s \right] \quad \text{(A8.6)}$$

For the calculation of X_{ds}, the suspending solids, an empirical equation is used (Morgan, 1986):

$$X_{ds} = 10^{-3} Y (E \exp(-aP))^b \qquad \text{(A8.7)}$$

In this equation, E, the kinetic energy of rainfall is calculated as follows (empirically):

$$E = 11.9 + 8.7 \log J \qquad \text{(A8.8)}$$

This formula gives the amount of kinetic energy per m^3 of rainfall per day.

Sedimentation of solids is assumed to occur due to gravity, only. Stokes' law is applied to calculate the falling velocity of a particle (assumed to be uniformly spherical) (De Greef and van de Meent, 1989):

$$\overline{V} = \frac{1}{18} \overline{d}_p^{\,2} g(\overline{\rho}_p - \rho_w) \frac{86400}{\eta} \qquad \text{(A8.9)}$$

The sine term with which the falling velocity is multiplied is to consider the influence of the horizontal velocity; α_z denotes the angle between the vector for horizontal velocity (q_r) and the resulting vector of horizontal and vertical (falling) velocity at height z. If α_z is large, i.e. when a particle comes close to the surface, the sine of α_z will approach the value of 1. Therefore, the influence of gravity will be larger near the soil surface, i.e., when z is small. This is illustrated in figure A8.3.

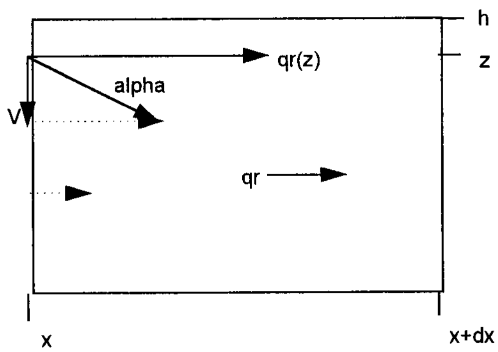

Figure A8.3. Vectors for horizontal and vertical movement of a suspended particle.

The dispersion coefficient is calculated from the dispersion coefficient for water (de Greef and van de Meent, 1989):

$$D_s = \gamma D_w \qquad \text{(A8.10)}$$

In this equation, gamma is the correction for interaction between particles:

$$\gamma = 1 + \left[\frac{X_s(z)}{X_s(\max)}\right]^{0.8} - 2\left[\frac{X_s(z)}{X_s(\max)}\right]^{0.4} \qquad \text{(A8.11)}$$

$X_s(z)$ is the local (at height z) sediment concentration, which is calculated by:

$$X_s(z) = X_s(w)\left[\left(\frac{w}{z}\right)\left(\frac{h-z}{h-w}\right)\right]^L \qquad \text{(A8.12)}$$

if w/h < 0.5, and:

$$X_s(z) = X_s(w)\left[\frac{w}{h-w}\right]^L \exp\left[-4L\left(\frac{z}{h}-0.5\right)\right] \qquad \text{(A8.13)}$$

if w/h >= 0.5.

For L, the suspension number, the following applies:

$$L = \frac{\overline{V}}{\kappa u_s} \qquad \text{(A8.14)}$$

In which u_s is the shear stress velocity at the soil surface:

$$u_s = \sqrt{gh(\tan\theta)} \qquad \text{(A8.15)}$$

Finally, D_w can be described with:

$$D_w = \left[\frac{0.4104}{\kappa^3} + \frac{\kappa}{6}\right] h u_s \qquad \text{(A8.16)}$$

Compounds

Compound in water

For the compound in water, the following differential equation can be derived (Bird et al., 1986):

$$\frac{\partial C_w}{\partial t} = -\frac{\partial F_w}{\partial x} - k_1 C_w + k_2 C_s X_s - \frac{I C_w}{h} \qquad \text{(A8.17)}$$

The dissolved compound flux, F_w, is assumed to consist of a convective part and a dispersive part (van Mazijk, 1983):

$$F_w = q_r C_w - D_c \frac{\partial C_w}{\partial x} \qquad \text{(A8.18)}$$

Substitution in equation A8.17 gives:

$$\frac{\partial C_w}{\partial t} = -\frac{\partial (q_r C_w)}{\partial x} + D_c \frac{\partial^2 C_w}{\partial x^2} - k_1 C_w + k_2 C_s X_s - \frac{I C_w}{h} \qquad \text{(A8.19)}$$

The (vertically averaged) dispersion coefficient for the compound in water, D_c, can be described with (de Greef and van de Meent, 1989):

$$D_c = (0.011)\frac{q_r^2 y^2}{hu_s} \qquad \text{(A8.20)}$$

Parameter q_r represents the vertically averaged fluid velocity (due to the shear stress, a velocity profile as in figure 3 is obtained).

Compound on suspended solids

For a compound on suspended solids, the following differential equation can be derived (Bird et al., 1960):

$$\frac{\partial(C_s X_s)}{\partial t} = -\frac{\partial(q_r C_s X_s)}{\partial x} + D_s \frac{\partial^2 (C_s X_s)}{\partial x^2} + k_1 C_w - k_2 C_s X_s + C_{ds} X_{ds} - \frac{\overline{V} \sin \alpha_z}{h} C_s X_s \qquad \text{(A8.21)}$$

Compound in settled (suspending) solids

For a compound in settled (suspending) solids, the following differential equation could be derived (Bird et al., 1960):

$$\frac{\partial(C_{ds} X_{ds})}{\partial t} = \frac{\overline{V} \sin \alpha_z}{h} C_s X_s - C_{ds} X_{ds} + k_3 C_w - k_4 C_{ds} \qquad \text{(A8.22)}$$

A8.3. Advantages and disadvantages

Currently, runoff decay is calculated in EUPHIDS fully empirical. Advantages are, that this method is fairly simple, also to implement into a system like EUPHIDS, and that data requirements are not very high. A drawback is, however, the large number of expert judgment assumptions.

The method proposed in this chapter is a mechanistic approach based on established theories of hydrodynamics, transport and sorption kinetics. This is an advantage compared to the currently implemented method. A disadvantage, however, is the larger data requirement and the larger complexity of the method. This complexity could have consequences for programming and implementing.

A8.4. Data-availability

With regard to the availability of parameters that are required as input, it can be stated, that most of the data required should not deliver too many problems. However, with regard to the data required for sorption, it could deliver some difficulties: In this proposal, it is assumed, that the sorption system is a one-site system, i.e. there is no intraparticulate diffusion or a rate-limiting site. Brusseau et al. (1990) and Boesten and van der Pas (1988) conclude that a one-site kinetics approach does not describe sorption properly, whereas a bicontinuum approach (two-site kinetics) is capable of proper prediction. It is assumed in this chapter, that equilibrium will not be reached due to the transport processes, and that the rate limiting site (intraparticulate site) is not relevant. Therefore, it is assumed, that one-site kinetics can be applied here. If this is possible, the desorption kinetic rate constant should be obtained from literature along with the sorption coefficient. Provided, that the equilibrium ratios do not change, the following is valid:

$$K_d = \frac{k_1}{k_2} \qquad \text{(A8.23)}$$

A8.5. Some final remarks

The formularium proposed here is meant merely to give a global view of the approach. Before this proposal can be implemented, there is a lot to be considered. Below, a brief list of topics to be considered is given:

Data collection
Solution of the differential equations
Programming
Sensitivity/Uncertainty analysis
Calibration/Validation

Notation

h = height of water column above soil (m)
q_r = fluid velocity (vertical average) (m/day)
x = horizontal length (m)
θ = slope angle of the runoff plane (°)
n = soil roughness (-)
R = daily precipitation (m/day)
I = infiltration rate (m/day)
K_{sat} = saturated hydraulic conductivity (m/day)
A = 'sorptivity', the slope of I vs. $t^{1/2}$
t = time (days)
X_s = content of suspended solids in water (kg/m3)
X_{ds} = settled solids/suspending solids (kg/m3 rainfall)
$\overline{V}$ = falling velocity of a (spherical) particle (particle size averaged) (m/day)
α_z = angle between horizontal (fluid) velocity and the resultant of horizontal (fluid) velocity and vertical (falling) velocity at height z (°)
F_s = sediment flux (kg/m2)
D_s = sediment dispersion coefficient (m2/day)
Y = soil detachability index (g/J)
E = kinetic energy of rainfall (J/m3day)
a,b = empirical constants; values often used are 0.05 and 1.0, respectively
P = percentage throughfall of precipitation (%)
J = rainfall intensity (m/h)

$\bar{d}$ = average diameter of a particle (m)
$\bar{\rho}_p$ = average (bulk) density of particles (kg/m3)
g = gravitational acceleration (m/s2)
ρ_w = density of water (kg/m3)
η = viscosity of water (Pa.s)
D_w = dispersion coefficient of water (m2/day)
γ = correction factor for particle interaction (-)
$X_s(z)$ = content of suspended solids in water at water column height $z<h$ (kg/m3)
$X_s(max)$ = maximum content of suspended solids in water, value often used = 0.65 (kg/m3)
w = reference water column height $w<z$ (m)
L = suspension number (-)
κ = von Karmann constant (-), mostly set at 0.4
u_s = shear stress velocity (m/day)
C_w = concentration of compound in water (kg/m3)
C_s = content sorbed on suspended solids (kg/kg)
F_w = compound flux (dissolved) (kg/m2day)
D_c = compound dispersion coefficient (m2/day)
k_1 = adsorption rate constant to suspended solids (1/day)
k_2 = desorption rate constant from suspended solids (1/day)
y = transversal width (m) = 1
C_{ds} = content sorbed on settled/suspended solids (kg/kg)
k_3 = adsorption rate constant to settled solids (1/day)
k_4 = desorption rate constant from settled solids (kg/m3day)
K_d = sorption coefficient (m3/kg).

PART THREE: Reference material

A9. List of publications and presentations

A9.1. Available publications

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