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EVALUATION SYSTEM FOR PESTICIDES (ESPE)

1. Agricultural pesticides

To be incorporated into the
Uniform System for the Evaluation of Substances (USES)

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SUMMARY

Since 1975 the Dutch Pesticide Act requires an evaluation of the hazards of pesticides, with regard to both public health and environment, before a pesticide is registered. Within this framework, the National Institute of Public Health and Environmental Protection (RIVM), in co-operation with the Support Group Environment of the Committee for the Registration of Pesticides (CTB), has developed an evaluation or risk assessment system for agricultural pesticides. This assessment system estimates the hazards for man and environment resulting from the use of these pesticides. The evaluation system has also been placed within the context of the Uniform System for the Evaluation of Substances (USES).

The evaluation system for pesticides (ESPE) is divided in three parts: 1) emission of the pesticide; 2) distribution over and within the different environmental compartments and calculation of exposure concentrations of organisms to the pesticide; 3) hazard assessment. The mathematical descriptions of various parts of the assessment system for agricultural pesticides are presented in this report.

In the first part, an estimation is made of the percentages of emission of the used dosage for the several environmental compartments. In the distribution part, the different transport and translation processes are assessed. This leads to Predicted (Initial) Environmental Concentrations (P(I)ECs) for the different environmental compartments and to transport fluxes between these compartments. In the third part, hazard assessment is carried out by comparing P(I)ECs with chronic or acute toxicity data (e.g. NOECs, L(E)C50s) for several non-target organisms. For the environmental hazard assessment decision trees, developed by the Support Group Environment of the CTB, are used. For human beings, in this system only consumers, no decision trees have been developed. Hazard assessment for indirect exposure is performed by comparing the total daily intake with the No Observed Adverse Effect Level (NOAEL).

SAMENVATTING

De Nederlandse Bestrijdingsmiddelen Wet vereist sinds 1975 een risicoevaluatie van bestrijdingsmiddelen voor mens en milieu, voordat deze stoffen toegelaten worden voor gebruik. In het kader hiervan is op het Rijksinstituut voor Volksgezondheid en Milieuhygiëne (RIVM), in samenwerking met de Steungroep Milieu van de Commissie Toelating Bestrijdingsmiddelen (CTB), een risico-beoordelingssysteem voor landbouwbestrijdingsmiddelen ontwikkeld. Met behulp van het beoordelingssysteem wordt een inschatting gemaakt van de mate van gevaar voor mens en milieu in relatie tot het gebruik van bestrijdingsmiddelen. Het systeem is tevens opgenomen in het project "Uniform Beoordelingssysteem Stoffen (UBS)".

Het beoordelingssysteem voor bestrijdingsmiddelen (BLN) is te verdelen in drie onderdelen:

1) emissie van het bestrijdingsmiddel; 2) verspreiding over en binnen de verschillende milieucompartimenten en berekening van de blootstelling van organismen aan het bestrijdingsmiddel; 3) risico-evaluatie. De wiskundige beschrijvingen van de verschillende onderdelen binnen het beoordelingssysteem voor landbouwbestrijdingsmiddelen worden in dit rapport gepresenteerd.

In het eerste onderdeel wordt een schatting gemaakt van het emissiepercentage van de toegepaste dosering naar de verschillende milieucompartimenten. In het verspreidingsonderdeel worden de verschillende transport- en omzettingsprocessen ingeschat. Dit leidt tot "Predicted (Initial) Environmental Concentrations (P(I)EC's)" voor de verschillende milieucompartimenten en tot transportfluxen tussen deze compartimenten. In het derde onderdeel worden risico-evaluaties uitgevoerd, door P(I)EC's te vergelijken met acute of chronische toxiciteitsgegevens (bv. NOEC's, L(E)50's) voor diverse organismen. Deze risico-evaluaties worden uitgevoerd met behulp van, door de Steungroep Milieu van de CTB ontwikkelde, beslisbomen. Voor de risico-evaluatie bij de mens, in dit systeem alleen consumenten, zijn geen beslisbomen opgesteld. Risico-evaluatie voor indirecte blootstelling vindt hier plaats door vergelijking van de totale dagelijkse inname met de "No Observed Adverse Effect Level (NOAEL)".

1. INTRODUCTION

1.1 General context

Since the Dutch Pesticide Act of 1962 came into effect, the evaluation of hazards of pesticides is required. Till 1975 this evaluation only concerned public health hazards. In 1975 the Pesticide Act was amended, and a hazard evaluation for the environment also became mandatory. The reason was that the authorities, responsible for the registration of pesticides, increasingly became aware of the consequences of continuous input into the environment of chemical substances, including pesticides. As a result of this amendment, the companies applying for registration of pesticides were now asked to submit environmental data too. Based on these data, pesticides, as well as their most important metabolites, are to be evaluated on their distribution and behaviour in the environment and on their effects to organisms in the environment. The evaluation should establish within sufficient certainty that by using the pesticide there will be no unacceptable harmful side-effects to the environment, to human beings (both consumers and employees), and to other organisms in the environment, as meant in art. 3 of the Pesticide Act.

1.2 Registration procedure

The general registration (notification) procedure for new agricultural pesticides is outlined in Figure 1. It has to be noticed, however, that this procedure will be changed per January 1993, after privatization of the Committee for the Registration of pesticides (CTB).

A company which intends to market a new pesticide must notify the competent authority. The competent authority in The Netherlands is the CTB. The Ministry of Housing, Physical Planning and Environment (VROM), the Ministry of Agriculture, Nature Management and Fisheries (LNV), the Ministry of Welfare, Public Health and Culture (WVC) and the Ministry of Social Affairs and Employment (SZW) take part in this Committee. Notifications must be accompanied by a limited base set of information (the content of the base set will be discussed in paragraph 1.3). The task of the National Institute of Public Health and Environmental Protection (RIVM) in this procedure is the evaluation of the base set information with respect to the environment and consumers. Principals are the ministries of VROM, LNV and WVC. The evaluation, which is coordinated by the Toxicology Advisory Centre (ACT), is performed in close collaboration with experts from other RIVM laboratories (Figure 2). The data evaluated are suitable for inclusion in the automated database of the ACT: TOXBANK (from 1993: TOXIS). Occupational health aspects are evaluated by the Dutch Organisation for Applied Scientific Research (TNO), in charge of the Ministry of SZW.

Environmental aspects of the final RIVM advisory reports are extensively discussed by the Support Group Environment (M) of the CTB. The Plant Protection Service (PD), the National Institute for Integrated Fresh Water Management and Waste Water Treatment (RIZA) and the RIVM are represented in here.

After approval by the Support Group M an evaluated summary of the relevant properties for the environment is directed via the Office for Pesticides (BB) into the CTB channels.

The Working Group Agriculture (L) reviews the advices on environmental aspects, on human

toxicological and consumers aspects, and on efficacy and occupational health aspects. In addition, it prepares the policy decision. The Ministry of LNV, the Ministry of VROM, the Ministry of SZW, the Ministry of Traffic and Public Works (V&W), and the Ministry of WVC take part in this Working Group.

The final advice is ratified by the CTB, after which a registration order is issued by the Minister of LNV.

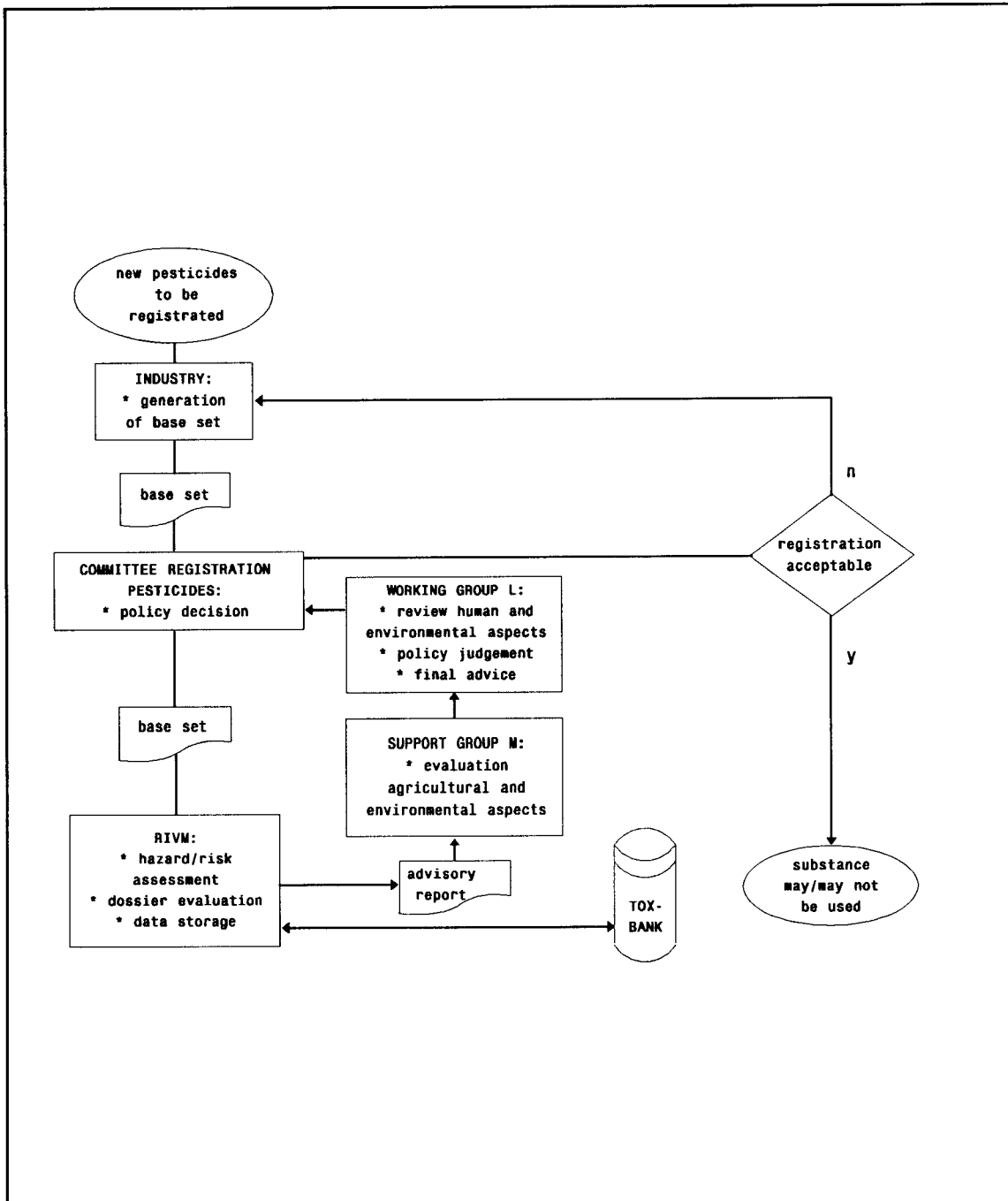


Figure 1. Simplified registration scheme of the procedure for the evaluation of pesticides.

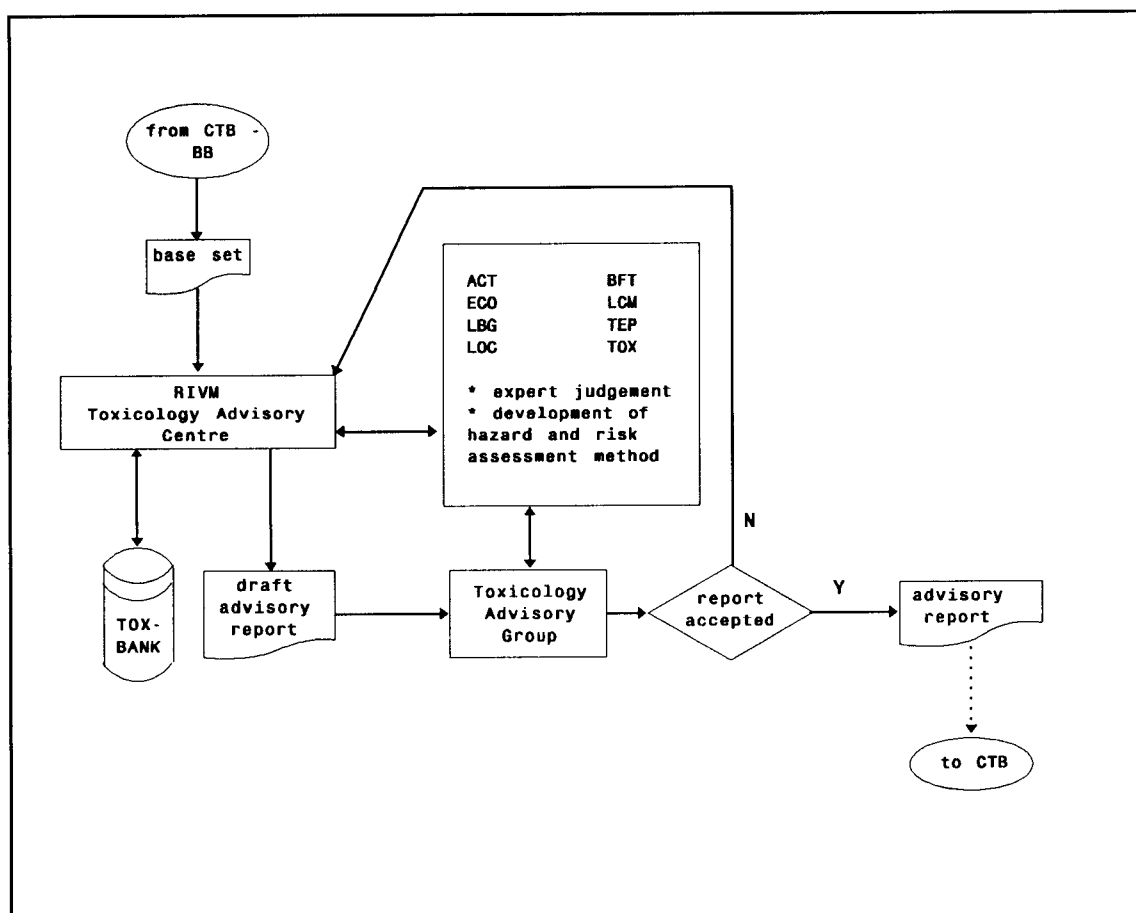


Figure 2. Instrumental RIVM procedures for evaluation of pesticides; BB = Office for Pesticides, CTB = Committee for the Registration of Pesticides, RIVM = National Institute of Public Health and Environmental Protection, ACT = Toxicology Advisory Centre, ECO = Laboratory of Ecotoxicology, LBG = Laboratory of Soil and Groundwater Research, LOC = Laboratory of Organic-Analytical Chemistry, BFT = Laboratory of Biotransformation, Farmaco- and Toxicokinetics, LCM = Laboratory of Carcinogenesis and Mutagenesis, TOX = Laboratory of Toxicology, TEP = Laboratory of Teratology, Endocrinology and Perinatal Screening.

1.3 Base set data

When giving notification of a new pesticide, supply of the base set of data is obligatory. A distinction is made into agricultural and non-agricultural pesticides (Figure 3). Agricultural pesticides are subdivided based on application method. Non-agricultural pesticides are subdivided based on function and usage, like disinfectants, wood preservatives, household applications and anti-fouling. Up to now, the base set of data required for non-agricultural pesticides is primarily based on the base set of agricultural pesticides. Some experience with non-agricultural pesticides shows that a more specific base set for these substances is required.

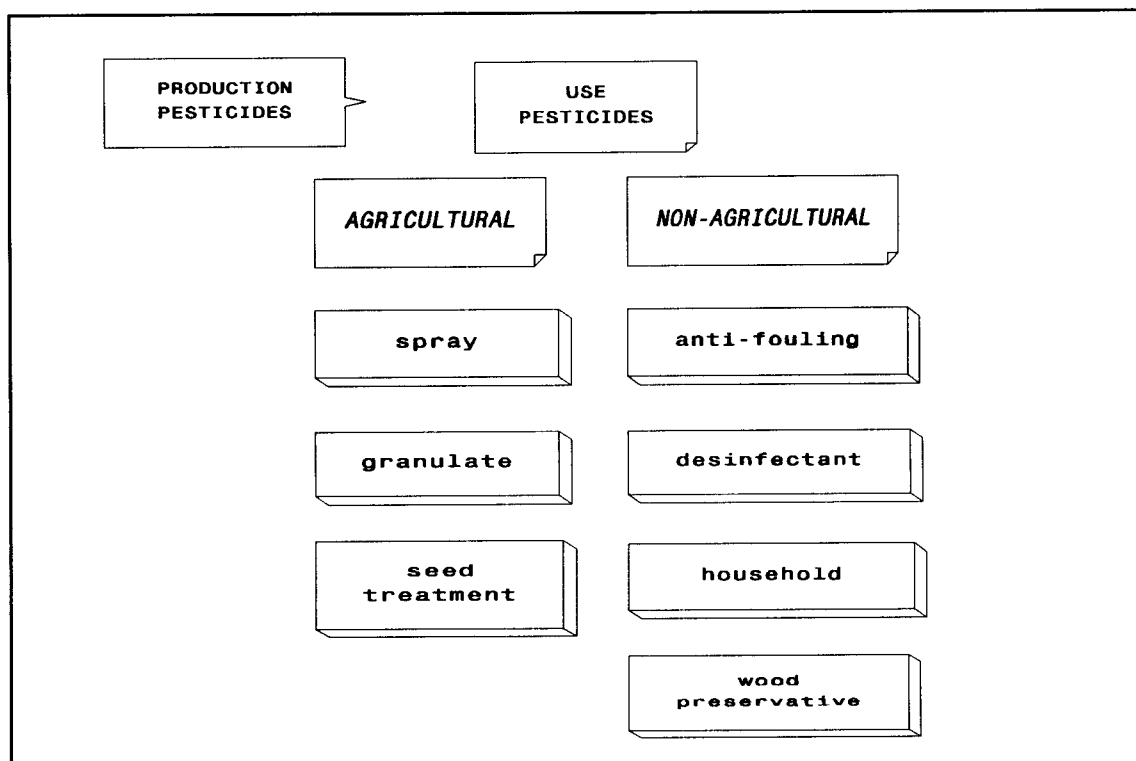


Figure 3. Distinction of pesticides.

The required base set data of agricultural pesticides is in agreement with regulations in other countries (e.g. Germany, Denmark and England) as much as possible. The data must refer to the active ingredient and its most important metabolites. However, if necessary, data of the formulation can be required. At the moment the base set consists of the following data:

- * Identity:
primary name, chemical names, trade names, CAS-number;
- * Properties:
structure and molecular weight, purity, additives and formulations, physical properties (appearance, melting point, boiling point, density, vapour pressure, surface tension, solubility in water, fat and other solvents, n-octanol/water partitioning coefficient), stability, spectra;
- * Analysis and detection:
methods;
- * Function and uses:
application, frequency, dosage;
- * Chemobiokinetics and metabolisms:
in animals, (humans) and plants;

- * Toxicology:
animal: acute toxicity, irritation, sensitization, subacute toxicity, semichronic toxicity, chronic toxicity and carcinogenicity, reproduction toxicity, teratogenicity, mutagenicity;
- * Ecotoxicology:
 - behaviour in soil: degradation, sorption and mobility;
 - behaviour in water: hydrolysis, photodegradation, biodegradation;
 - toxicity for organisms:
 - # birds: acute and subacute studies;
 - # waterorganisms: freshwater studies (short term and long term);
 - # insects: bees;
 - # soil-organisms: micro-organisms and enzymes in soil and manure, earthworms;
 - bioaccumulation;
- * Residues:
crop, contamination of food and drinking water.

1.4 Environmental evaluation of base set data

Canton *et al.* (1991) have presented an overview of the evaluation of ecotoxicological data of about 150 agricultural pesticides. During the evaluation of this number of pesticides the need for a consistent and reproducible evaluation procedure became evident. More standardization of assumptions and situations took place. The Support Group M of the CTB started several subgroups on specific topics in the environmental evaluation procedure, like behaviour in soil, behaviour in water, and toxicity for waterorganisms. The proposals of these subgroups finally led to the development of decision trees for nine different subjects (CTB, 1992):

- leaching to shallow ground water
- contamination of surface water
- hazard to water organisms
- hazard to earthworms
- hazard to nitrification
- hazard to birds and mammals
- hazard to bees
- hazard to 'beneficial organisms':
 - * *Encarsia formosa* (an ichneumon fly)
 - * *Phytoseiulus persimilis* (a predatory mite)

Except for the evaluation of hazards to beneficial organisms all subjects mentioned were part of the evaluation of the 150 pesticides (Canton *et al.*, 1991). In the underlying report the subjects are linked together to form an assessment system for pesticides. Therefore, the base set is completed by setting standard assumptions for environmental parameters. This report describes in detail the assumptions and parameter values needed for this assessment system.

2. HAZARD ASSESSMENT FOR AGRICULTURAL PESTICIDES

2.1 Introduction

In general, pesticides are introduced into the environment through emissions during use. From this point, the compounds will be distributed in the environment. Not only target organisms, but also non-target organisms will be exposed, and therefore undesirable side-effects may occur on some species, communities or on ecosystems as a whole (Toet *et al.*, 1991).

In order to determine the hazard for potential adverse effects for human beings and other organisms in the environment, an evaluation or risk assessment system for pesticides has been developed. The system is meant to screen these potential hazards, given the limited number of base set data and makes use of specific insights in emission and distribution of chemicals. Meanwhile, the risk assessment system is also incorporated into the second prototype of the Uniform System for the Evaluation of Substances (USES), next to the assessment system for new chemicals and a prioritization system for existing chemicals (DRANC and PRISEC). To maximize the harmonization between the three assessment systems, the same configuration as in the risk assessment system for new and existing chemicals is used as much as possible.

The terms "hazard" and "risk" are used as internationally agreed (EC, 1990):

Hazard is defined as the potential of a substance to cause adverse effects at a particular degree of exposure. Risk is defined as the probability that these adverse effects actually occur.

2.2 Basic philosophy

The basic philosophy of the risk assessment system is already described by Toet *et al.* (1991). The risk assessment system for pesticides is also based on causality between emissions and effects: emissions cause concentrations in the environment, which can cause effects on organisms, communities or ecosystems and on human beings:

Emission --> Distribution --> Concentrations --> Exposure --> Effects

This chain is outlined in Figure 4.

The assessment of exposure includes the estimation of emissions into the environmental compartments, and the distribution of emitted substances over the different compartments of the environment. The results of the exposure assessment are Predicted Environmental Concentrations (PECs) and an estimation of the total daily intake by human beings.

The effect assessment starts with the available toxicity data, e.g. LC50, EC50 or NOEC values for aquatic and terrestrial organisms and a No Observed Adverse Effect Level (NOAEL) for mammals. The actual hazard assessment takes place by a comparison of the degree of exposure with no-effect levels. The quotient of the Predicted Environmental Concentration and the No Effect Concentration (PEC/NEC) is an indication of the hazard that direct exposure may cause effects. The quotient of the total daily intake (or "Predicted Environmental Dosage" (PED)) and the NOAEL (margin of safety) is an indication of the hazard for man.

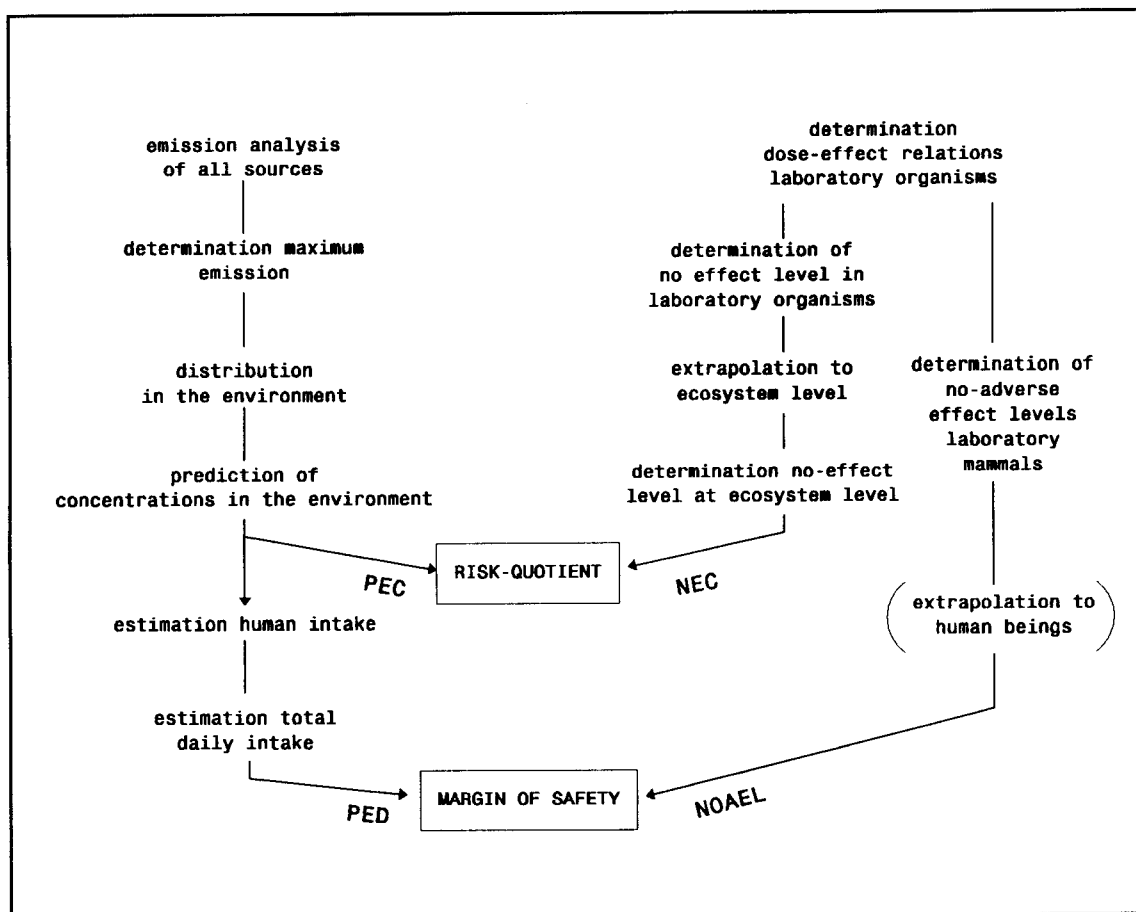


Figure 4. The causality chain between emissions and effects; the chain in the risk assessment system.

2.3 Limitations

Limitations of the evaluation system are caused by:

- the number of data provided in the notification of pesticides;
- the availability of correct model descriptions.

Although the amount of data in the base set of pesticides is more extensive than before the amendment of 1975, it still does not provide all the data necessary to cover all hazards. Therefore, not every route of exposure can be taken into consideration. In addition, the wide variety in pesticides, pesticide uses, pesticide formulations, and environmental conditions makes it impossible to analyze all hazards. Therefore, assumptions and simplifications are needed to fill data gaps and to make the assessments generally applicable. When an application of a pesticide is very specific, e.g. in the cultivation of mushrooms, a hazard assessment suitable for that situation will be performed if hazards are expected.

When the amount of data provided is limited, assumptions, estimations, and extrapolation methods are used to generate an indicative value for the unknown parameter, process or no-effect level. If additional data become available, generally a better hazard assessment can be carried out.

Often simplified model descriptions are used to describe the complex processes of distribution of the compound within the environment and the ultimate exposure of organisms. However, these simplifications also account for the limitations of these models. The available base set of data also limits the choice of useful model descriptions. In addition, many model descriptions have been developed for specific chemicals under specific conditions. Reliable relations between characteristics of a very broad range of chemicals and environmental behaviour are scarce (Toet *et al.*, 1991).

2.4 Uncertainty and natural variance

To avoid underestimation of potential hazards, a worst case approach might be followed, by using the highest possible emissions, worst case compound parameters, and vulnerable environmental conditions. However, this approach would result in unrealistic high hazards, and all substances would be qualified as highly hazardous. This is not the intention of the risk assessment system, which is meant to estimate realistic hazard levels for pesticides. The method chosen during the development of the risk assessment system is to assume 'realistic worst case' conditions, implying the quantification of realistic values for variables and parameters and uncertainties and variances of these variables and parameters (Toet *et al.*, 1991).

Although *uncertainty* is one of the keywords in hazard assessment, it is not yet taken into account in this report. However, it is a fact that there is uncertainty in the estimation of emissions, distributions, and effects of these substances. Uncertainty will be included in the hazard assessment model in 1993-1994.

Variance is a term which is of even greater importance in the hazard assessment system. The assessment system is a reflection of 'the environment'. In reality, the environment shows an enormous diversity of environmental and meteorological conditions in time and space. A model must explicitly make major simplifications in this diversity. These simplifications are the origin of large variances in variables.

Uncertainties and variances may lead to an over- or underestimation of actual hazards of pesticides. One of the main efforts in the development of the evaluation system for pesticides is to quantify the uncertainty and variance in the estimated values.

2.5 The evaluation system for pesticides

The evaluation system for agricultural pesticides is characterized by the underlying assumptions. The actual mathematical process descriptions can be found in chapter 3. The starting points are:

- * The system is to be used in The Netherlands. Therefore, the environmental and meteorological conditions are defined, in accordance with Dutch circumstances.
- * The system assumes an agricultural soil with a standard area of 1 ha, surrounded by ditches with a length of 100 m, a width of 2 m and a depth of 0.25 m.

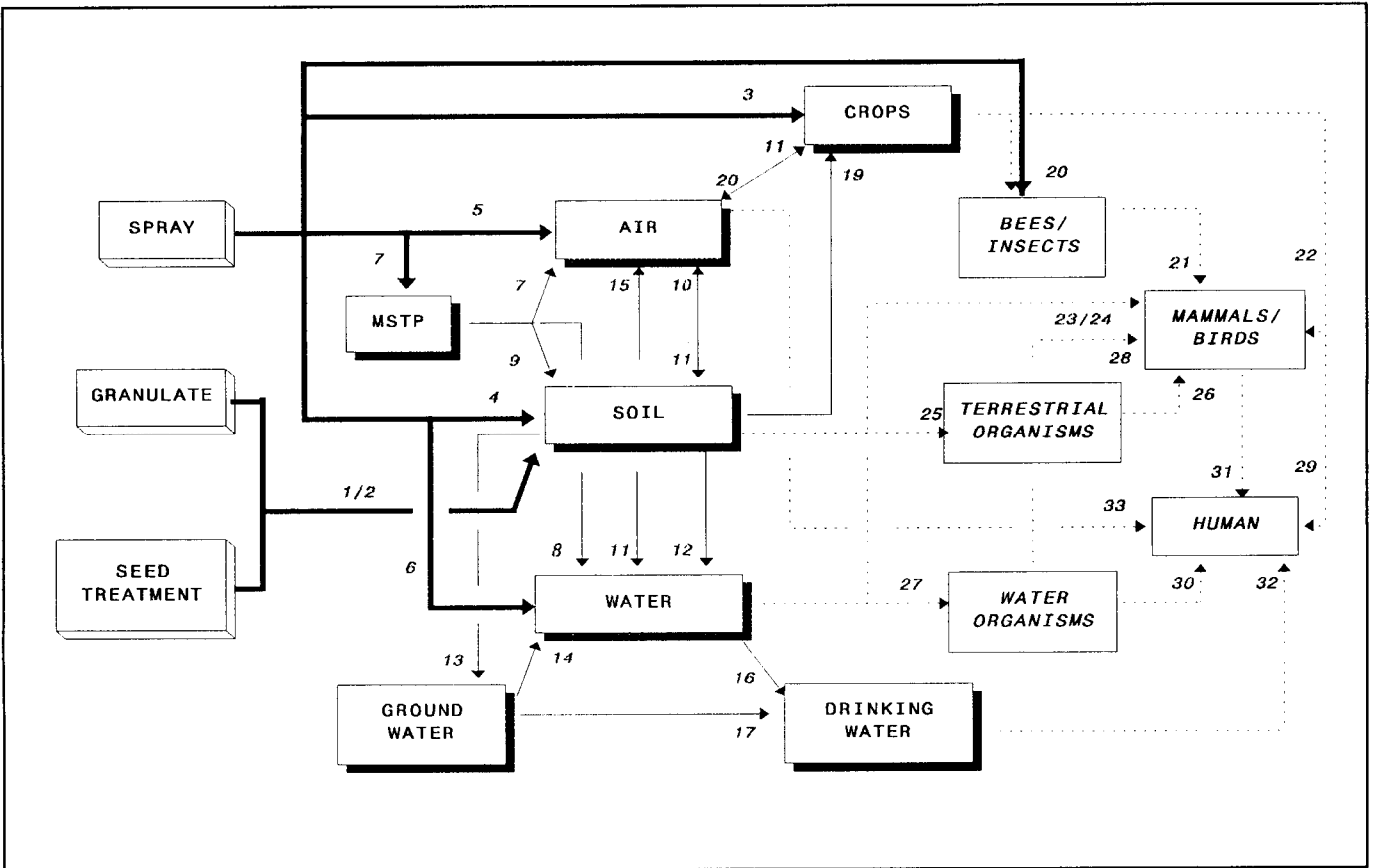
- * The system is based on the decision trees developed by the CTB (1992). Additional developments are taken into account after approval by the CTB.
- * The exposure assessment is carried out on a local scale, but not site-specific. The local scale is defined as the near surroundings of the main source of a substance after application. Instead of an actual site, a hypothetical site is defined with average environmental characteristics for The Netherlands.
- * Emission of pesticides starts with an application according to Good Agricultural Practice (GAP). In Figure 5a the routes of exposure considered in the system are indicated. Other routes are possible but they are omitted in this stage, because:
 1. a model description is not yet known in the literature, or
 2. the route is considered to be of negligible importance, unless in future the opposite will be proven.
- * Environmental hazard is generally expressed by means of the ratio $P(I)EC/NOEC$, which means that a Predicted (Initial) Environmental Concentration ($P(I)EC$), calculated according to the exposure analysis, is compared to the No Observed Effect Concentration ($N(O)EC$). Besides the $P(I)EC$ and $NOEC$, also other exposure data, like the Predicted Environmental Dose (PED) and acute toxicity data, like the $L(E)C50$, are used.
- * Hazard assessment for human beings is only concerned with indirect exposure via the consumption of food and drinking water, and the inhalation of air. Hazard is expressed by means of the ratio Total Daily Intake / No Observed Adverse Effect Level ($NOAEL$).

It has to be noticed that the evaluation system for pesticides is not meant to give an exact mass-balance of the fate of a pesticide in the environment. Aim is to obtain an indication of the most important distribution and exposure routes, so that attention can be focused on these routes.

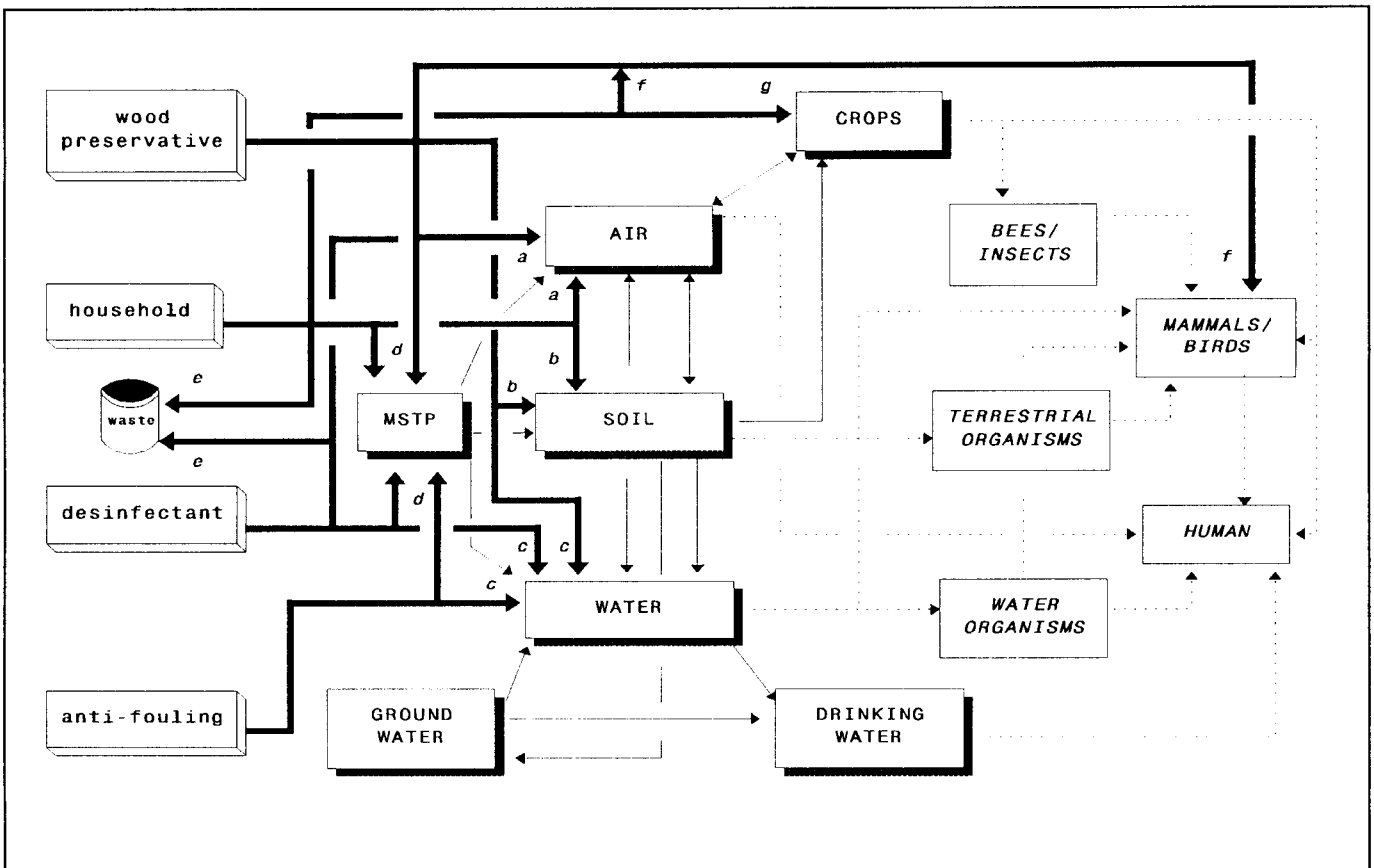
In Figure 5 the routes of the evaluation system for both agricultural and non-agricultural pesticides are presented.

As can be seen in Figure 5a the scheme of the agricultural system can be divided into three parts: emission, distribution and hazard assessment.

- The emission part describes the various routes via which the pesticide enters the environment after agricultural use. The production process of pesticides or formulations is explicitly excluded from this evaluation system.
- The distribution part describes the physical-chemical processes by which the pesticide is transported through the environment. Final goal of these routes is the calculation of PECs for water, drinkwater, air, soil, and sludge.
- The hazard assessment part describes the comparison of calculated exposure concentrations with toxicity data for the organisms exposed, by means of decision trees, which are developed by the CTB (CTB, 1992).

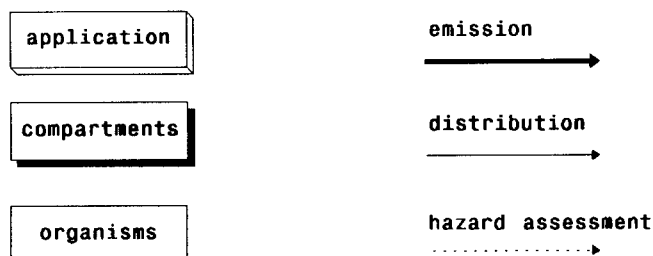


5a.



5b.

Figure 5. a: The various routes for application of agricultural pesticides. The numbers in the figure refer to part II of this report: description of routes. M.s.t.p. = municipal sewage treatment plant.
 b: The various routes for application of non-agricultural pesticides; a = emission to air, b = emission to soil, c = emission to water, d = emission via m.s.t.p., e = waste rest, f = exposure of bats/exposure via bioaccumulation, g = emission to crops.
 Legenda:



Each of the three parts consists of several routes. They are numbered in Figure 5a. The routes have the following meaning:

Emission:

1. Application of granulate on soil
2. Application of treated seed on soil
3. Application of sprays: interception by crops
4. Application of sprays: part that reaches the soil
5. Advection of sprays by the atmosphere
6. Drift to surface water
7. Discharge via settling tank on municipal sewage treatment plant

Distribution:

8. Discharge from m.s.t.p. into surface water and dilution
9. Deposition of sludge from m.s.t.p. on soil
10. Volatilization from the soil
11. Atmospheric deposition on soil, crops and surface water
12. Run-off and erosion to surface water
13. Leaching to ground water
14. Drainage
15. Volatilization from surface water
16. Surface water used for drinking water
17. Leaching to ground water used for drinking water
18. Volatilization from crops
19. Uptake by crops

Hazard assessment:

20. Exposure of bees and insects
21. Uptake of insects by birds and mammals
22. Uptake of crops by birds and mammals
23. Uptake of soil (granules or treated seeds) by birds and mammals
24. Uptake of water by birds and mammals
25. Exposure of and uptake by terrestrial organisms (e.g. earthworms) and effects on nitrification
26. Uptake of terrestrial organisms by birds and mammals
27. Exposure of and uptake by water organisms
28. Uptake of water organisms by birds and mammals
29. Consumption of crops by man
30. Consumption of fish by man
31. Consumption of meat and milk by man
32. Intake of drinking water by man
33. Inhalation of air by man

As can be seen in Figure 5b there are great similarities between the routes of application for agricultural and non-agricultural pesticides. It has to be noticed, however, that Figure 5b is not complete; more application and exposure routes should be added. In this report only the system for agricultural pesticides is dealt with in detail. In a following report, which will be published in 1993, the complete evaluation system for non-agricultural pesticides will be elaborated.

3. DESCRIPTION OF ROUTES

In this chapter the various routes of the evaluation system for agricultural pesticides will be described one by one. If possible, assumptions, restrictions, input and output data, and model calculations of each route will be presented. Input data will be classified in four groups:

- C Constants;
- R (Required) values from the notification dossier of a pesticide;
- E Expert estimations;
- O Output from previous models/calculations.

3.1 Emission

Three methods by which agricultural pesticides can be applied are considered: spraying liquids, granules and seed treatments (see figure 5a). A certain compound can have several forms, so that more than one application method is possible. Then, all application methods concerned should be followed.

The dosage in which the pesticide will be used should be supplied by the applicant (Table 1).

Table 1. Application of pesticides

Output	Symbol	C/R/E/O
Dosage (kg a.i./ha).	Dos	R

Route 1. Application of granules on soil.

It is possible, although not likely, that a granule application is repeated during the season. If this is the case, the maximum concentration, reached during the season, should be calculated. The maximum concentration is dependent on the half-lifetime for biodegradation, the application frequency, and the interval between two applications. With the help of Appendix 1 it can be calculated as presented in Table 2.

Table 2. Method for calculating maximum granule concentration after repeated application

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Single dosage (kg a.i./ha)	Dos	R
Half-life for biodegradation (d)	DT50	R
Application frequency (-)	n	R
Application interval (d)	l	R
Output		
Apparent maximum dosage (kg a.i./ha)	Dos _{max}	

Model calculation:

From Appendix 1 the ratio Dos_{max}/Dos can be obtained (Dos_{max} = amount of pesticide after n applications), from which the Dos_{max}-value can be derived.

If the application frequency (n) = 1, then Dos_{max} = Dos.

Granules can be mixed with the soil or left at the soil surface. If mixed it is considered that only 1% of the applied dose is left at the soil surface. If not mixed this is considered to be 100% (Table 3).

Table 3. Model for mixing granules with soil

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Apparent maximum dosage (kg a.i./ha)	Dos _{max}	O
Factor for mixing with soil (-)	F _{mix} = 0.01	C
Factor for not mixing with soil (-)	F _{notmix} = 1.0	C
Output:		
Dosage of granules on soil surface (kg a.i./ha)	Dos _{sur}	

Model calculations:

Pesticide dose at surface when mixed with soil

$$\text{Dos}_{\text{sur}} = F_{\text{mix}} * \text{Dos}_{\text{max}}$$

Pesticide dose at surface when not mixed with soil

$$\text{Dos}_{\text{sur}} = F_{\text{notmix}} * \text{Dos}_{\text{max}}$$

It is assumed that granules, if mixed with the soil, are distributed homogeneously over the top 20 cm of soil. If not mixed, a distribution over the top 5 cm is assumed for calculations. The soil is assumed to have a bulk density of 1400 kg/m³. With these assumptions the Predicted Initial Environmental Concentration (PIEC), in mg a.i./kg soil, can be calculated (Table 4). This PIEC is considered to be equal to the concentration on day 0 (C_0 or $C_{\text{soil.tot}}$), which is used in several models.

Table 4. Calculation of the Predicted Initial Environmental Concentration (PIEC)

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Maximum dosage (kg a.i./ha)	Dos_{max}	O
Depth of soil (m):	H_{soil}	C
if mixed with soil	0.2	
if not mixed with soil	0.05	
Bulk density (kg/m ³)	$B_d = 1400$	C
Output:		
Predicted Initial Environmental Concentration (mg a.i./kg)	$C_{\text{soil.tot}}$ or PIEC	
Model calculation:		
$PIEC = Dos_{\text{max}} * 10^6 / (10^4 * H_{\text{soil}} * B_d)$		

It should be noticed that the total amount of pesticides in the soil is distributed between solids (the solids related concentration, C_{soil}) and soil water (the dissolved concentration, $C_{\text{soil.wat}}$):

$$PIEC \text{ or } C_{\text{soil.tot}} = C_{\text{soil}} + C_{\text{soil.wat}}$$

This distribution is dependent on the distribution coefficient ($K_{s/l}$). The dissolved and the solids related concentration can be calculated as follows (Table 5):

Table 5. Calculation of dissolved and solid related concentrations in soil

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Total concentration in soil (mg a.i./kg)	PIEC (or $C_{\text{soil.tot}}$)	O
Distribution coefficient (dm ³ /kg)	$K_{s/l}$	R
Bulk density (kg/m ³)	$B_d = 1400$	C

(to be continued)

Table 5. (continued)

Parameter/variable (unit)	Symbol
Output:	
Dissolved concentration (mg a.i./l)	$C_{\text{soil.wat}}$
Solids related concentration (mg a.i./kg)	C_{soil}
Model calculations:	
<i>Dissolved concentration</i>	
$C_{\text{soil.wat}} = C_{\text{soil.tot}} / (1 + K_{\text{s/l}})$	
<i>Solids related concentration</i>	
$C_{\text{soil}} = C_{\text{soil.tot}} * (K_{\text{s/l}} / (1 + K_{\text{s/l}}))$	

Route 2. Application of treated seed on soil.

When treated seeds are brought on the soil, they can be mixed with the soil or left at the soil surface. As with granules, it is considered that 1% of the applied dose is left at the soil surface when the seeds are mixed with the soil. Otherwise this is considered to be 100% (Table 6). Treated seeds are not applied more than once during one season, hence the applied dosage (Dos) is similar to the maximum dosage (Dos_{max}).

Table 6. Model for mixing treated seeds with soil

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Dosage (kg a.i./ha)	Dos	R
Factor for mixing with soil (-)	$F_{\text{mix}} = 0.01$	C
Factor for not mixing with soil (-)	$F_{\text{notmix}} = 1.0$	C
Output:		
Dosage of seed treatment on soil surface (kg a.i./ha)	Dos _{sur}	

(to be continued)

Table 6. (continued)**Model calculations:***Pesticide dose at surface when mixed with soil*

$$\text{Dos}_{\text{sur}} = F_{\text{mix}} * \text{Dos}$$

Pesticide dose at surface when not mixed with soil

$$\text{Dos}_{\text{sur}} = F_{\text{notmix}} * \text{Dos}$$

The PIEC can be calculated in the same way, with the same assumptions and input data, as with granules (Route 1; Table 4):

$$\text{PIEC} = \text{Dos} * 10^6 / (10^4 * H_{\text{soil}} * B_d) \quad (\text{mg a.i./kg})$$

The dissolved concentration and the solids related concentration can be calculated according to the method described in Table 5. In this way it is assumed that the compound is distributed evenly in the soil after sowing.

Routes 3 + 4. Application of sprays on soil: interception by crops and part that reaches the soil.

Sprays are regularly applied more than once during a season. Therefore the maximum dosage should be calculated according to the method described in Table 2.

After a pesticide has been sprayed, a part of it is intercepted by crops. The rest reaches the soil or the surface water, or disappears into the air. It is assumed that the most regular spraying methods are used. The fraction of the dosage that reaches the soil together with the fraction that is intercepted by the crop is supposed to be **90%** (leaving 10% for air-emission). In Table 7 an overview is presented of the part of the spraying-liquid that is intercepted by crops or that reaches the soil (depending on the crop and growing stage). In Table 8 the model is presented for calculating the soil concentration after interception, assuming a homogeneous distribution over the relevant soil depth of 5 cm.

Table 7. Part of spraying-liquid that is intercepted by the crop (P_{int}) or reaches the soil (P_{soil})

Crop and growing stage	Target	% Intercepted by the crop (P_{int})	% On the soil (P_{soil})
Potatoes, beets, 2-4 weeks after emergence	insects	20%	70%
Potatoes, beets, full growth	plant louses potato disease	80%	10%
Apple trees, in spring	1st scab-spray	40%	50%
Apple trees, full foliage	from 3rd scab-spray	70%	20%
Peas, short after emergence	insects	10%	80%
Peas, around bloom	insects, fungi	70%	20%
Corns, 1 month after emergence	a.o. weeds	10%	80%
Corns, full growth	fungi	80%	10%
Grassland	weeds, insects	40%	50%
Sprouts, full growth	insects	70%	20%
Onions, full growth	fungi	50%	40%
Default		10%	80%

Table 8. Model for interception of spray by the crop

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Apparent maximum dosage (kg a.i./ha)	Dos_{max}	O
Interception by the crop (%)	P_{int}	E/C
Percentage on the soil (%)	P_{soil}	E/C
Depth of soil (m)	$H_{soil} = 0.05$	C
Bulk density (kg/m ³)	$B_d = 1400$	C
Output:		
Dosage intercepted by crops (kg a.i./ha)	Dos_{int}	
Dosage that reaches the soil (kg a.i./ha)	Dos_{soil}	
Concentration of spray in soil (mg a.i./kg)	$C_{soil,tot}$ or PIEC	

Model calculations:*Interception by the crop*

$$Dos_{int} = Dos_{max} * P_{int}/100$$

Part that reaches the soil

$$\text{Dos}_{\text{soil}} = \text{Dos}_{\text{max}} * P_{\text{soil}}/100$$

Distribution over soil layer

$$\text{PIEC} = \text{Dos}_{\text{soil}} * 10^6 / (10^4 * H_{\text{soil}} * B_d)$$

The dissolved concentration and the solids related concentration can be calculated according to the method described in Table 5.

Route 5. Advection by the atmosphere.

For determining the advection through the atmosphere the OPS-model (Operating Priority Substances model), described by Van Jaarsveld (1990) can be used. One of the main characteristics of the OPS-model is that it does not describe specific short-term pollution events, but it estimates long-term averaged concentrations and deposition fluxes caused by continuous emissions.

The following scales for exposure through air are used:

- For the estimation of concentrations in air, it is chosen to use concentrations at the border of an agricultural site, which is assumed to be at 100 meter from the source.
- The deposition of a substance (route 11) on local soils is assumed to take place in a circle with a radius of 1 km around the point source, representing the local agricultural area.

The input parameters of the OPS-model can be categorized in *source characteristics, substance characteristics, and environmental characteristics.*

For the various *source characteristics* default values are presented in Table 9 (see also Toet & De Leeuw, 1992).

Table 9. Default values for source characteristics

Parameter/variable (unit)	Symbol	Default Value
Source strength (g/s)	S.str.	1.0
Source height (m)	S.hei.	10
Source diameter (m)	S.dia.	0
Heat content of the plume (MW)	H.con.	0

A source strength of 1 g/s indicates an emission of 86.4 kg pesticide per day, which is extremely high. Therefore, this default value should be adapted by correcting for the actual amount of emission per day:

Actual S.str. = Default S.str * (Actual emission/day / default emission/day (= 86.4 kg))

The parameters which are needed for the OPS-calculations and are dependent on *substance characteristic* are presented in Table 10.

Table 10. Substance characteristics and parameters needed for OPS-calculations

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Octanol-water partition coefficient (-)	K_{ow}	R
Vapour pressure (Pa)	V_p	R
Aerosol surface (m^2/m^3)	$\theta = 5 \cdot 10^{-3}$	C
Constant (Pa*m)	$c = 0.2$	C
Henry coefficient ($Pa \cdot m^3/mol$)	H	R
Gas constant (J/(mol*K))	$R = 8.3$	C
Absolute temperature (K)	T	C
Output parameters used for calculation:		
Ratio between gaseous and aerosol-bound substances (-)	ϕ	
Washout ratio (-)	W	
Dry deposition velocity (cm/s)	V_d	
Reaction rate in the atmosphere (%/h)	K_r	

Estimation methods:

Ratio between gaseous and aerosol-bound substances

$$\phi = (c * \theta) / (V_p + c * \theta)$$

Washout ratio

$$W = H / (R * T)$$

Dry deposition velocity

$$V_d = 0.01 \text{ cm/s (range: } 1 \cdot 10^{-3} - 1 \text{ cm/s)}$$

Reaction rate

$$K_r = 5 \text{ %/h (range: 0 - 100%/h)}$$

The *environmental characteristics* important for the OPS-model are the distance of receptor points from the source, the surface roughness of the source area, and the meteorological conditions.

The distance from the source is given by the assumed exposure areas: 100 m for concentrations and 1 km for deposition.

For assumptions on the roughness length and the meteorological conditions, see Toet *et al.* (1991).

The final calculation of the OPS-model, the concentration at a distance of 100 m from the source (in $\mu\text{g}/\text{m}^3$), is split up in two parts:

1. Calculation for gaseous substances;
2. Calculation for aerosol-bounds substances.

Route 6. Drift to surface water.

A part of the applied dosage of a sprayed pesticide reaches the surface water directly. The concentration in the surface water as a result of this drift can be calculated with the so called 'SLOOT.BOX-model'. This model takes into account repeated dosage and several environmental processes, like biodegradation, volatilization, advection, sedimentation and resuspension, and calculates short-term and long-term Predicted Environmental Concentrations (PECs). Further details, assumptions, and default-values are presented by Linders *et al.* (1990). The way in which the pesticide is applied has a great influence on the amount of drift. De Jong (1991) has estimated the amount of drift as a function of way and place of treatment (Table 11). In this table percentages of the original dosages are presented that are sprayed on non-target areas. In the evaluation system the non-target area is a ditch with a mean depth of 0.25 m.

Table 11. Percentage drift related to place and way of application

Location and way of application	P _{drift} (%)
1. Indoor applications ¹ (excl. greenhouses)	
- storage cells, etc.	0
- shower rooms, etc.	0
2. Protected applications	
a. Specific applications	
- overhead irrigation	0
- manual pouring	0
- soil treatment	0
- granule application	0
- trickling	0
- chicory for silage	0
b. Non-specific applications	
- remaining ways of application in greenhouses (spraying, mist blowing, fogging, smoke generating, etc. : mainly through condensation on glass roof) ²	0.1

(to be continued)

Table 11. (continued)

Location and way of application	P _{drift} (%)
3. Field applications:	
a. Specific applications:	
- manual pouring	0
- dipping	0
- granule application ³	0
- baiting	0
- injecting soil/plant	0
- treating plant base	0
- smearing	0
- brushing	0
- spraying with direct incorporation into soil ⁴	0
- seed treatment	0
b. Spot applications:	
- waste dump	0.5
- row spraying ⁵	0.5
- knapsack spraying	0.5
- road signs	0.5
c. Non-specific applications:	
1. crop height < = 25 cm ⁶ :	
- soil treatment	1
- bare soil	1
- herbicide in fruit culture	1
- under-leaves spraying	1
- plant bed	1
- before germination	1
- paved terrain	1
2. crop height > 25 cm:	
- downward spraying	2
- treatment field border	5
- edge along ditch slope	5
- sideways or upward directed spraying in arbori- and fruit culture	10
3. ditch slope application	10
d. Specific applications:	
- spraying by aircraft	100
- willow-coppice	100
- dry ditch bottom	100

¹ Whenever no direct exposure of surface water by drift is to be expected by the way of applying, the load through this route is determined to be 0%.

² From research into condensate discharge, it was derived that approximately 0.1% of the plant protection products dosage on the glass roof can load the surface water via condensate. Up to now, it has been impossible to explicate per way of application.

³ With special synthesis granule broadcasting device.

⁴ Spraying with direct incorporation into the soil during a sole run of labour.

⁵ This figure is based on the assumption, that during row spraying less drift will occur than during field application, as the distance from nozzle to soil is substantially less during row spraying than during whole field treatments.

⁶ During applications on 'bare soil' and (still) low crops a relatively low emission is assumed as a result from the possibility to adjust the spraying boom closer over the crop on the field.

Concentrations of pesticides in surface water as a result of drift ($C_{\text{wat.drift}}$) can be calculated as follows:

$$C_{\text{wat.drift}} = \text{Dos (kg a.i./ha)} * P_{\text{drift}}/100 / \text{Depth of ditch}$$

$$= \text{Dos (mg/dm}^2) * P_{\text{drift}}/100 / 2.5 \text{ (dm)} \quad (\text{mg/l})$$

This concentration is similar to the short term Predicted Environmental Concentration ($PEC_{\text{short-term}}$), the concentration in the surface water a few days after application, which is calculated with SLOOT.BOX. Besides, SLOOT.BOX also calculates the concentration in surface water direct after application ($C_{\text{wat.0}}$) and the concentration in surface water after about one year, the $PEC_{\text{long-term}}$.

For the behaviour of pesticides in water a decision tree has been drawn up (CTB, 1992; see Appendix 3). Input data of this decision tree are:

- Half-lifetime for biodegradation in municipal sewage treatment plant ($DT50_{\text{mstp}}$) (d) R
- Half-lifetime for photodegradation in surface water ($DT50_{\text{phot}}$) (d) R
- Half-lifetime for hydrolysis in surface water ($DT50$) (d) R
- Half-lifetime for biodegradation ($DT50_{\text{biodeg}}$) (d) R
- K_p -value (dm^3/kg) R
- Predicted Environmental Concentration ($PEC_{\text{short-term}}$) (mg a.i./l) O
(calculated with SLOOT.BOX-model)

Route 7. Discharge via settling tank on municipal sewage treatment plant.

In some cases it is possible that a pesticide reaches a municipal sewage treatment plant (m.s.t.p.) via a settling-tank (for example with the culture of mushrooms). According to Jobsen (1988), a fixed dilution factor for the settling tank of 10 can be applied (Table 12).

Table 12. Model for discharge on settling tank

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Dosage (kg a.i./ha)	Dos	R
Application frequency (per cel of 200 m ²)	$F_{\text{app}} = 1$	C
Number of cells (-)	$n = 5$	C
Emission percentage (%/24 h)	$P_{\text{emm}} = 4$	C
Waste water flow rate (m ³ /24 h/installation of 1000 m ²)	$Q = 1.5$	C
Dilution factor for settling-tank (-)	$F_{\text{dil}} = 10$	E/C

(to be continued)

Table 12. (continued)**Output:**

Amount of compound used per cel of 200 m ² (kg/cel)	Dos _{cel}
Effluent concentration of settling-tank (mg a.i./l)	C _{eff.st}

Model calculation:

Amount of compound used per cel

$$\text{Dos}_{\text{cel}} = 200/10000 * \text{Dos} = 0.02 * \text{Dos}$$

Effluent concentration

$$C_{\text{eff.st}} = (n * F_{\text{app}} * \text{Dos}_{\text{cel}} * (P_{\text{emm}}/100) * 10^6) / (Q * F_{\text{dil}} * 1000) = 0.27 * \text{Dos}$$

The effluent of the settling tank will be transported to a municipal sewage treatment plant and then discharged into the surface water. This process has originally been modelled by Struijs *et al.* (1987, 1991), and is fully described by Toet *et al.* (1991). The model is based on a multicompartimental Mackay Level III fugacity model (Mackay & Paterson, 1982).

In a municipal sewage treatment plant a pesticide can be removed by biodegradation. Dependent on the octanol-water partition coefficient it may sorb onto suspended solids (sludge particles). Volatilization may occur if the Henry coefficient is higher than $1 \cdot 10^{-5}$ Pa·m³/mol. Transport occurs through advection (water flow, sludge flow), diffusion (into sludge particles or into the bottom sediment), sedimentation and volatilization.

The model of the municipal sewage treatment plant consists of 9 compartments between which the transport processes take place. The model has the following output data (Toet *et al.*, 1991):

Table 13. Output of m.s.t.p.-model

Parameter/variable (unit)	Symbol
Effluent concentration, dissolved (mg a.i./l)	C _{eff.dis}
Effluent concentration, particular (mg a.i./l)	C _{eff.abs}
Effluent concentration, total (mg a.i./l)	C _{eff.tot}
Concentration in sludge produced (mg a.i./kg)	C _{sludge}
Volatilization from m.s.t.p. (kg a.i./d)	Vol _{m.s.t.p.}

3.2 Distribution

Route 8. Discharge from m.s.t.p. into surface water and dilution.

The effluent of the m.s.t.p. is discharged into recipient water. This process has been modelled by Toet *et al.* (1991) and is presented in Table 14. Two processes take place in the recipient water:

- dilution, modelled by means of a median dilution factor;
- adsorption on or desorption from suspended solids, dependent on the (calculated) partition coefficient.

Eventually, also precipitation may take place, in case the dissolved concentration exceeds the solubility by more than a factor 10.

Table 14. Surface Water Module

Variable/parameter (unit)	Symbol	C/R/E/O
Input:		
Octanol/water partition coefficient (-)	K_{ow}	R
Solubility in water (mg/l)	S_{wat}	R
Effluent concentration (mg a.i./l)	$C_{eff.tot}$	O
Dilution factor (-)	F_{dil}	E/C
Concentration suspended solids (mg/l)	C_{sus}	E/C
Fraction organic carbon in susp. sol. (-)	F_{oc}	E/C
Output:		
Sediment/water partition coefficient (dm ³ /kg)	$K_{sed-wat}$	
Dissolved surface water concentration (mg a.i./l)	$C_{wat.dis}$	
Total surface water concentration (mg a.i./l)	$C_{wat.tot}$	

Model calculations:

Dilution

$$C_{wat.tot} = C_{eff.tot} / F_{dil}$$

Sediment/water partitioning (according to DiToro et al., 1991)

$$K_{sed-wat} = 1.0 * K_{ow} * F_{oc}$$

$$C_{wat.dis} = C_{wat.tot} / (1 + K_{sed-wat} * C_{sus} * 10^{-6})$$

Precipitation

if $C_{\text{wat.dis}} > 10 * S_{\text{wat}}$:

correct or do not correct the concentration to $10 * S$ (optional, program asks for Yes or No).

Route 9. Application of sludge from m.s.t.p. on soil.

Besides the direct applications of pesticides (routes 1-4), distribution of pesticides to soil may take place by means of the use of the sludge of the m.s.t.p. as fertilizer on arable land or grassland. Concentrations in the soil are the result of mixing the toplayer of the soil with an amount of sludge (Table 15). The application of sludge should be seen apart from the direct applications of granules, treated seeds or sprays. After application, the evaluation system should be followed from route 10.

Table 15. Application of sludge on soil

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration in dry sludge from m.s.t.p. (mg a.i./kg)	C_{sludge}	O
Dilution factor agricultural soil (-)	$F_{\text{mix.a}} = 0.2$	C
Dilution factor grassland soil (-)	$F_{\text{mix.g}} = 0.05$	C
Output:		
Concentration in agricultural soil (mg a.i./kg)	$C_{\text{a.soil}}$	
Concentration in grassland (mg a.i./kg)	$C_{\text{g.soil}}$	

Model calculations:

$$C_{\text{a.soil}} = C_{\text{sludge}} * F_{\text{mix.a}}$$

$$C_{\text{g.soil}} = C_{\text{sludge}} * F_{\text{mix.g}}$$

Route 10. Volatilization from the soil.

A part of the dosage that has reached the soil volatilizes. This process can be modelled according to Van de Meent *et al.* (1992):

Table 16. Model for volatilization from the soil

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Depth of soil (m)	H_{soil} (0.05/0.20 m)	C
Octanol/water partition coefficient (-)	K_{ow}	R
Vapour pressure (Pa)	V_p	R
Solubility in water (mol/l)	S_{wat}	R
Time (d)	t	C
Concentration of pesticide in soil at day 0 (mg a.i./kg)	PIEC	O
Output:		
First order transport rate constant for volatilization (-)	$K_{\text{vol}}(\text{soil})$	
Concentration of pesticide in soil at day t (mg a.i./kg)	$C_{\text{soil},t}$	
Half-lifetime (d)	DT_{50}	

Model calculations:*Transport rate constant*

$$K_{\text{vol}}(\text{soil}) = 1/H_{\text{soil}} * (1.9*10^4 + 2.6*10^4 * K_{\text{ow}}/(P_v/S_w))$$

First order concentration decrease

$$C_{\text{soil},t} = \text{PIEC} * e^{-K_{\text{vol}}(\text{soil}) * t}$$

$$DT_{50} = [H_{\text{soil}} * (1.9*10^4 + 2.6*10^4 * K_{\text{ow}}/(P_v/S_w))] * \ln 2$$

Route 11. Atmospheric deposition on the soil, surface water and crops.

Deposition on soil, surface water and crops can be calculated with the OPS model, developed by Van Jaarsveld (1990). The assumptions and the input parameters of the model have already been discussed at route 5.

As with advection, the final calculation of this model, the deposition flux averaged over a circle with a radius of 1 km (in $\text{g}/\text{m}^2 \cdot \text{s}$), is split up in two parts:

1. calculations for gaseous substances;
2. aerosol-bound substances.

Route 12. Run-off and erosion to surface water.

Besides volatilization and percolation into the root zone and connected soil layers, horizontal transport can take place, i.e. run-off and erosion. The mathematical models for run-off and erosion fluxes are described by De Greef (1992). The models assume that run-off and erosion are calculated under circumstances that represent a soil with an average uniform vegetation cover and directly following application of a pesticide. The soil is in an average moisture condition prior to the application. Interception and water losses as result of evapotranspiration and evaporation are assumed not to contribute significantly to the amount of water that is available for transport over land. The pesticide is distributed instantaneously between the soil matrix and moisture; the precipitation starts shortly after the moment of application. Finally, conservation management practices, such as tillage, aimed at reduction of run-off and erosion are not taken into account.

In Table 17 the model for run-off is presented.

Table 17. Model for calculation of run-off

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Length of parcel (m)	L = 100	C
Width of parcel (m)	W = 100	C
Elevation (m)	EI	C
Frequency peak storm depth (m)	q _p = 0.05	C
Watershed cover (-)	C	C
Concentration in soil water (g/cm ³ = 10 ⁶ mg/l)	C _{soil.wat}	O
Run-off Curve Number (-)	RCN	C
Output:		
Flow time (h)	T _c	
Rainfall rate (cm/d)	Q _s	
Peak storm run-off (cm/d)	Q _p	
Initial abstraction (cm/d)	I _a	
Potential infiltration (cm/d)	S	
Run-off depth (cm/d)	Q _r	
Run-off flux (mg/d)	J _r	

Model calculations*Flow time*

$$T_c = L^{1.15} / (7700 * EI^{0.38})$$

Rainfall rate

$$Q_s = q_p / (T_c * a)$$

(a = 24; conversion from h to d)

Peak storm value

$$Q_p = C * Q_s * W * L$$

(Dutch situation: C = 0.2)

Potential infiltration

$$S = 1000 / RCN - 10$$

(Dutch situation: RCN = 81)

Initial abstraction

$$I_a = 0.2 * S$$

Run-off depth

$$Q_r = (Q_p - 0.2*S)^2 / (Q_p + 0.8*S)$$

Run-off flux

$$J_r = Q_r * C_w * W * L$$

In Table 18 the model for erosion is presented. In general, it can be assumed that the significance of erosion can be disregarded for those pesticides which exhibit apparent distribution coefficients, K_d , of less than or equal to 5.0.

Table 18. Model for calculation of erosion

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Length of parcel (m)	L = 100	C
Width of parcel (m)	W = 100	C
Run-off depth (cm/d)	Q_r	O
Percentage silt or fine sand (%)	P_1	C
Percentage sand (%)	P_2	C
Soil organic matter (%)	a	C
Soil structure code (-)	b = 2	C
Permeability class (-)	c = 4	C
Soil cover factor (-)	$F_{cov} = 1$	C
Conservation practice factor (-)	$F_{con} = 1$	C
Concentration of pesticide on soil solids (mg a.i./kg)	C_{soil}	O

(to be continued)

Table 18. (continued)

Output:	
Run-off volume (m ³ /d)	V_r
Peak storm value (cm/d)	Q_p
Soil erodibility factor (-)	F_{er}
Particle size diameter (mm)	M
Slope steepness factor (-)	F_{sl}
Factor m (-)	$m = 0.2^a$
Soil loss from erosion (t/d)	Q_e
Erosion flux (g/d)	J_e
Enrichment factor for organic matter (g/g)	r_{om}

Model calculations:*Run-off volume*

$$V_r = Q_r * W * L$$

Particle size diameter

$$M = (P_1 + (100 - P_2)) / 100$$

Soil erodibility factor

$$K = (2.1 * 10^{-6}) * M^{1.14} * (12-a) + 3.25 * (b-2) + 2.5 * (c-3)$$

Slope steepness

$$F_{sl} = (L/72.6)^m * (65.41 * \sin^2(EI/L) + 4.56 * \sin(EI/L) + 0.065)$$

Soil loss from erosion

$$Q_e = a * (V_r * Q_p)^{0.56} * F_{er} * F_{sl} * F_{cov} * F_{con} \quad a = 1.4$$

Distribution coefficient for organic matter

$$\ln(r_{om}) = 2 + 0.2 * \ln(Q_e/A)$$

Erosion flux

$$J_e = Q_e * r_{om} * C_{soil}$$

(to be continued)

^a the factor m can be determined by means of the percentage elevation (e ; $e = EI/L \cdot 100$):

$$e \geq 5.0 \quad \rightarrow \quad m = 0.5$$

$$3.5 \leq e \leq 4.0 \quad \rightarrow \quad m = 0.4$$

$$1.0 < e < 3.0 \quad \rightarrow \quad m = 0.3$$

$$e \leq 1.0 \quad \rightarrow \quad m = 0.2$$

In the Dutch situation generally $e < 1$, therefore $m = 0.2$

Because run-off and erosion coincide, the total flux of pesticide to surface water is the sum of the respective fluxes:

$$J_t = J_r + J_e \quad (\text{g/d})$$

It is assumed that run-off and erosion are acute processes and take place in 1 day. The standard ditch used in this evaluation system has a length of 100 m, a width of 2 m, and a depth of 0.25 m, giving a total volume of $50 \text{ m}^3 = 50000 \text{ dm}^3$. In this way the concentration in the surface water as a result of run-off and erosion can be calculated.

$$C_{\text{wat.r/e}} = J_t \cdot \text{Time (d)} / \text{Vol (dm}^3) = J_t \cdot 1 / 50000 \quad (\text{g/dm}^3)$$

Route 13. Leaching to ground water.

An estimation of leaching to ground water is made on the basis of the rate of conversion of a pesticide and its mobility (Support Group M model: PESTLA; Van der Linden & Boesten, 1989). The model is based on the following assumptions:

- Soil type: relatively vulnerable sandy soil. The organic matter content is determined to be 4.7% in the A_p horizon (0-30 cm) and 0.8% and 0.2% in the lower B_3 and C_{11} horizons (30-50 cm and 50-59 cm, respectively); the C_{12} horizon (110-120 cm) contains 0.1%.
- Soil treatment: none (untilled soil). After applying a pesticide, the soil is not ploughed or otherwise tilled so that displacement of the substance through mixing of soil layers is excluded.
- Culture: maize (important for evaporation, evapotranspiration).
- Dosage: a single spring or autumn application of 1 kg a.i./ha, that reaches the soil.
- Precipitation: data from a 75% wet year (gross precipitation in 74% of the years is lower).

In Table 19 the in- and output data of the PESTLA-model are presented.

Table 19. Input and output of PESTLA-model

Variable	Symbol	C/R/E/O
Input:		
Adsorption coefficient (dm ³ /kg)	K _{om}	R
Half-lifetime for biodegradation (d)	DT50	R
Output:		
Modelled conc. in shallow groundwater (mg a.i./m ³)	C _{gw(model)}	
Leaching from upper one meter of soil (% of dosage)	L	
Residue in plough layer after 1 year (% of dosage) ^a	Res	

^a The absolute concentration in µg/kg in the plough layer (the upper 20 cm of the soil) is calculated assuming a soil density of 1400 kg/m³. The conversion factor of 3.6 thus obtained is rounded to 4, giving C_{soil} = 4 * Res (µg a.i./kg soil).

The output values can be obtained by graphs or by means of computer calculations. In Appendix 2 the values are calculated for various combinations of DT50 and K_{om}.

Remark

The original output graphs present the results in the Kom - DT50 area of 0 - 200, 0 - 200. For use in the evaluation system this area is extended to 0 - 500, 0 - 500 by calculating additional grid points. All the calculated grid points in the area 0 < DT50 < 500 and 0 < Kom < 500 are used to interpolate the value of the estimated ground water concentrations, the leaching to ground water and the remaining amount in the upper soil layer after logarithmic transformation.

Because the PESTLA-model assumes a dosage of 1 kg a.i./ha, the concentration in the shallow groundwater should be corrected for the actual applied dosage:

$$C_{gw} = \text{Dos}_{\text{max(calc)}} * C_{\text{gw(model)}} / \text{Dos}_{\text{(model)}}$$

in which:

Dos_{max(calc)} = actual, calculated dosage (see routes 3,4, and 6)

C_{gw(model)} = concentration in shallow groundwater calculated with PESTLA

Dos_(model) = dosage assumed by PESTLA (being 1 kg a.i./ha)

C_{gw(model)} = actual concentration in shallow groundwater

For determining the hazard of leaching to shallow groundwater, a decision tree has been drawn up by the CTB (1992) (see Appendix 4).

In the future volatilization from the soil will be incorporated in the PESTLA-model.

Route 14. Drainage.

After the pesticide has reached the shallow groundwater via leaching (see route 13), there are two possibilities:

- Drains are present;
- Drains are not present.

In case there are no drains, it is assumed that all the pesticide disappears to the groundwater or drinking water (route 17), assuming conservative behaviour in the saturated zone. This gives the same concentration as calculated according to PESTLA.

In case there are drains, it is assumed that 40% of the pesticide disappears to the ground water (route 17) and that 60% is drained to the surface water. The concentration of the pesticide in the drains (C_{drai}) is similar to the concentration in the shallow ground water, but will decrease after the dilution by surface water.

Table 20. Model for calculating concentration in surface water after drainage

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Factor for dilution of drainage water (-) that reaches the surface water (-)	$F_{\text{dil}} = 0.1$	C
Concentration in shallow ground water (mg a.i./m ³)	C_{gw}	O
Output:		
Conc. in drainage water (mg a.i./l)	C_{drai}	
Conc. in surface water as result of drainage (mg a.i./l)	$C_{\text{wat.drai}}$	

Model calculations:

Concentration in drainage water

$$C_{\text{drai}} = C_{\text{gw}}$$

Concentration in surface water as result of drainage

$$C_{\text{wat.drai}} = 0.1 * C_{\text{drai}}$$

It is assumed that drainage is a chronic process. Therefore, the concentration in the surface water as a result of drainage should not be added to the Initial Concentration as a result of drift.

Route 15. Volatilization from surface water.

Volatilization from surface water can be described with the model of Liss & Slater (1974) (Table 21). In this model the main water body is assumed to be well mixed, with a thin layer on the surface in which there is a concentration gradient. The air above is assumed to be well mixed (i.e. the background level is assumed to be low), and a thin layer, in contact with the surface, contains another concentration gradient. At the interface between these two layers there is a concentration discontinuity, and the ratio of concentrations across it (air to water) is assumed to equal the Henry's law constant.

Transfer through these films is by straightforward molecular diffusion. The molecules are assumed to diffuse through the layers at a rate dependent on the phase exchange coefficients found in the equations rather than vaporize directly from solution along with the water vapour. This method is used in the SLOOT.BOX-model.

Table 21. Volatilization model according to Liss & Slater (1974)

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration in water at t=0 (g/cm ³) ^a	C _{wat.0}	O
Time (d)	t	C
Mean depth of the water body (cm)	Depth ^b	C
Henry's coefficient (Pa*m ³ /mol)	H	C
Temperature (K)	T	C
Gas constant (Pa*m ³ /(mol*K))	R	C
Gas-phase exchange coefficient (cm/s)	k _g ^c	C
Liquid-phase exchange coefficient (cm/s)	k _l ^c	C
Output:		
Non-dimensional Henry's law constant (-)	H'	
Overall mass transfer coefficient water phase (-)	K _l	
Conc. in water after volatilization during t days (g a.i./cm ³)	C _{wat.t}	
Half-lifetime volatilization (d)	t _{1/2}	
Conc. in air after volatilization during t days (g a.i./cm ³)	C _{air.t}	

Model calculations:

Non dimensional Henry's law constant

$$H' = H / (R * T)$$

Overall mass transfer coefficient water phase

$$1 / K_l = 1 / k_l + 1 / (H' * k_g)$$

Water concentration

$$C_{\text{wat.t}} = C_{\text{wat.0}} * e^{-K_1 * t / \text{Depth}}$$

$$t_{1/2} = 0.69 * \text{Depth} / K_1$$

Assuming an equilibrium at time t between the liquid-phase and the gas-phase the concentration in the gas-phase can be calculated by means of the Ostwald solubility coefficient (α'):

$$C_{\text{wat.t}} / C_{\text{air.t}} = 1 / \alpha' = 1 / H'$$

$$C_{\text{air.t}} = C_{\text{wat.t}} * H' \quad (\text{g a.i./cm}^3)$$

^a 1 mg a.i./l = $1 * 10^{-6}$ g a.i./cm³

^b In SLOOT.BOX model, depth of water body is 25 cm

^c Calculated in SLOOT.BOX model in m/d; 1 m/d = 0.0012 cm/s, so calculated k_g and k_l should be multiplied by 0.0012.

Route 16. Surface water used for drinking water.

The drinking water module has originally been described by Hrubec & Toet (1992). In this route it is assumed that water entering the surface water via the m.s.t.p. is used for drinking water. Therefore, the concentration of the pesticide is dependent on the concentration in the effluent water of the m.s.t.p. after dilution (route 8).

The model assumes a complete removal of suspended particles from the surface water. Removal of the dissolved fraction of a pesticide is modelled by means of a purification factor. This factor is based on simple physico-chemical substance properties, namely:

- K_{ow} ;
- Henry-coefficient;
- Aerobic biodegradation.

The various treatment processes are distinguished in:

- Dune recharge;
- Open storage;
- Coagulation, flocculation, or rapid sand filtration;
- Ozonization;
- Slow sand filtration.

The drinking water model is described in Table 22.

Table 22. Drinking water module

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Dissolved surface water concentration (mg a.i./l)	$C_{\text{wat.dis}}$	O
Purification factor (-)	$F_{\text{pur}}^{\text{a}}$	E
Output:		
Concentration in drinking (mg a.i./l)	$C_{\text{dr.wat}}$	

Model calculation:

Concentration in drinking water

$$C_{\text{dr.wat}} = C_{\text{wat.dis}} * F_{\text{pur}}$$

^a For F_{pur} values is referred to Hrubec & Toet (1992).

Route 17. Leaching to ground water used for drinking water.

As already described in route 14 (drainage) there are two possibilities after the pesticide has reached the shallow groundwater:

- Drains are present;
- Drains are not present.

If there are drains it is assumed that only 40% of the net precipitation will leach to the groundwater. If there are no drains 100% of the net precipitation will leach to the groundwater. However, the concentration in the groundwater will always be the same as in the shallow groundwater. This will give the following model:

Table 23. Model for leaching to groundwater

Variable/parameter (unit)	Symbol	C/R/E/O
Input:		
Concentration in shallow ground water (mg a.i./m ³)	C_{gw}	O
Output:		
Concentration in drinking water (mg a.i./l)	$C_{\text{dr.wat}}$	

(to be continued)

Table 23. (continued)**Model calculation:**

$$C_{\text{dr.wat}} = C_{\text{gw}} / 1000$$

It is possible to take into account transformation in the saturated zone. This transformation is depending on the transformation coefficient (k_{ts}). Assuming that the transformation coefficient equals the hydrolysis rate coefficient and that the process will take place following first order kinetics, this will give the following relationship:

$$C_{\text{gw.t}} = C_{\text{gw.0}} * e^{-k_{\text{ts}}*t} \quad (\text{mg a.i./m}^3)$$

$$\text{where: } k_{\text{ts}} = k_{\text{hydrolysis}} = \ln 2 / \text{DT50}_{\text{hydrolysis}}$$

and

$$C_{\text{dr.wat}} = C_{\text{gw.t}} / 1000 \quad (\text{mg a.i./l})$$

Dilution is not taken into account.

Route 18. Volatilization from crops.

The National Institute of Applied Scientific Research, TNO, has developed a method for calculating pesticide volatilization from crops (Huygen *et al.*, 1986ab). The model is designed to calculate the evaporative flux in the period immediately following treatment. It is therefore suitable for computing peak concentrations and deposition rates. An assumption is that only compounds left on the crop evaporate (for interception by crops, see route 3). The model is presented in Table 24.

Table 24. Model for volatilization from crops.

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Maximum dosage (kg a.i./ha)	Dos_{max}	O
Interception by crops (%)	P_{int}	C
Droplet radius (m)	$R_o = 0.2 * 10^{-3}$	C
Compound concentration in spray solution (kmol/m ³)	C_o	R
Vapour pressure (Pa)	V_p	R
Gas constant (J/(kmol*K))	$R = 8300$	C

(to be continued)

Table 24. (continued)

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Temperature (K)	T = 293	C
Laminar thickness (mm)	l = 0.03*10 ⁻³	C
Molecular Weight (kg/kmol)	M	R
Output:		
Initial evaporation flux (kmol/(m ² *s))	Flux _{eva}	
Dosage corrected for interception (kmol/m ²)	Dos _{int}	
Evaporation density (kmol/(m ² *s))	E _d	
Diffusion coefficient (m ² /s)	D	

Model calculations:*Diffusion coefficient*

$$D = 8.8 \cdot 10^{-9} \cdot (R \cdot T / M)^{2/3}$$

Evaporation density

$$E_d = D \cdot V_p / (R \cdot T \cdot l)$$

Dosage corrected for interception

$$Dos_{int} = (Dos_{max} \cdot P_{int}/100) / (M \cdot 10000)$$

Initial evaporation flux

$$Flux_{eva} = (3 \cdot Dos_{int} \cdot E_d) / (2 \cdot R_o \cdot C_o)$$

Route 19. Uptake by crops.

Besides volatilization, a part of the dosage can be taken up by crops. This uptake is modelled according to findings of Briggs *et al.* (1982, 1983). As reported by De Nijs & Vermeire (1990), a Stem Concentration Factor (SCF), a bioconcentration factor from transportation stream solution in a plant to concentration in stem tissue, can be calculated. Concentration in the transportation stream can be calculated by means of a Transport Stream Concentration Factor (TSCF) which links the concentration in the soil solution to concentrations in the transportation stream. The TSCF can be estimated, according to Briggs *et al.* (1982,1983), by means of the octanol/water partition coefficient.

Table 25. Model for uptake by plants

Variable	Symbol	C/R/E/O
Input:		
Concentration in soil (mg a.i. /kg)	PIEC	O
Fraction organic carbon in soil (-)	F _{oc}	C
Soil water content (-)	F _{sw}	C
Soil bulk density (g/cm ³)	R _{ho}	C
Octanol/water partition coefficient (-)	K _{ow}	C
Output:		
Organic carbon distribution coefficient (-)	K _{oc}	
Concentration soil solution (mg a.i./kg)	C _{soil.wat}	
Transportation stream concentration factor (-)	TSCF	
Stem concentration factor (-)	SCF	
Concentration in vegetable crops (mg/kg)	C _{crops}	
Concentration in grass (mg/kg)	C _{grass}	

Model calculations:*Sediment water partition*

$$\log K_{oc} = 0.989 * \log K_{ow} - 0.346$$

$$C_{soil.wat} = R_{ho} / (R_{ho} * K_{oc} * F_{oc} + F_{sw}) * PIEC$$

Plant uptake

$$TSCF = 0.748 * e^{-(\log Kow - 1.78)^2 / 2.44}$$

$$SCF = 0.82 + 10^{0.95 * \log Kow - 2.05}$$

$$C_{crops} \text{ and } C_{grass} = SCF * TSCF * C_{soil.wat}$$

3.3 Hazard assessment

Water and soil organisms are exposed to pesticides in various ways. For making a hazard assessment for these organisms, decision trees are drawn up by the CTB (1992). In these decision trees, exposure data (e.g. dosage, PIEC, PEC, PED), which are calculated in the previous routes, are compared with acute and chronic toxicity data. The lowest LC50 or NOEC value per group of organisms (mammals, birds, waterorganisms) is used. Extrapolation methods, which calculate a NOEC for a total group of organisms, taking into consideration the number of available toxicity data, are not applied.

In the decision trees four different risk¹ classifications for pesticides are distinguished:

- * No risk;
- * Low risk;
- * Intermediate risk;
- * High risk;

The various routes in which organism are exposed and the input data of the corresponding decision trees for hazard assessment are discussed in the next section. The decision trees themselves are presented in Appendices 5 - 13.

For the exposure routes of human beings, no decision trees have been developed. Hazard assessment for indirect exposure is performed in agreement with Toet *et al.* (1991)

Route 20. Exposure of bees and insects.

The decision trees for bees and insects are presented in Appendices 5 - 7. Decision trees are available for bees (Appendix 5), and for two 'beneficial insects', namely *Encarsia formosa*, an ichneumon fly (Appendix 6), and *Phytoseiulus persimilis*, a predatory mite (Appendix 7). The decision trees have the following input data:

Bees

- | | |
|---|---------------|
| - No Observed Effect Level (NOEL) from bees breeding-test | R |
| - Lethal Dose for 50% (LD50) of the organisms
in contact/oral test (mg a.i./kg, µg a.i./bee) | R |
| - Toxicity data from cage-test | R |
| - Toxicity data from field test | R |
| - Dosage (mg a.i./kg) | O (route 3/4) |

Encarsia formosa

- | | |
|--|---|
| - Data from residue toxicity test | R |
| - Toxicity data from direct contact test | R |
| - Toxicity data from persistence test | R |
| - Toxicity data from field test | R |

¹ Although "hazard" is meant, the term "risk" is used in the decision trees.

Phytoseiulus persimilis

- Data from residue toxicity test R
- Toxicity data from persistence test R
- Toxicity data from field test R

Routes 21 + 22. Uptake of insects or crops by birds and mammals.

The decision tree for the hazard assessment of birds and mammals after uptake of sprayed crops or insects, is presented in Appendix 8, module C. The decision tree is developed after research by Luttik (1993).

The decision tree has the following input data:

- LD50 (mg a.i./kg bw) R
- LD50_{species of concern} (mg a.i./species of concern) R
- LC50 (mg a.i./kg feed) R
- No Observed Effect Concentration (NOEC_{bird/mammal}; mg a.i./kg feed) R
- Predicted Environmental Concentration in Feed
(PEC_{feed short/long}) (mg a.i./kg feed) O
- Daily Feed Intake (g/day) C

The LD50_{species of concern} is similar to the LD50-value corrected for the mean weight of the bird- or mammal species:

$$\text{LD50}_{\text{species of concern}} = \text{LD50} * \text{mean weight target group}$$

By means of the average daily amount of feed (Daily Feed Intake; DFI) of birds and mammals, the Predicted Environmental Dose (PED_{DFI}), the dosage of an applied pesticide on the crops/insects that a bird or mammal can ingest per day (corrected for the DFI) can be calculated. The DFI for birds and mammals is strongly correlated to the body weight (BW). Nagy (1987) has derived the following relationships:

All birds

$$\log \text{DFI} = -0.188 + 0.651 * \log \text{BW} \quad (\text{g/d})$$

Passerines

$$\log \text{DFI} = -0.4 + 0.85 * \log \text{BW} \quad (\text{g/d})$$

Non passerines

$$\log \text{DFI} = -0.521 + 0.751 \log \text{BW} \quad (\text{g/d})$$

All mammals

$$\log\text{DFI} = -0.629 + 0.822 * \log\text{BW} \quad (\text{g/d})$$

The PED_{DFI} can then be calculated as follows:

$$\text{PED}_{\text{DFI}} = \text{PEC}_{\text{feed}} * \text{DFI} \quad (\text{kg/d})$$

Two derivations of the PEC_{feed} are also used in the decision trees:

- The $\text{PEC}_{\text{feed,short}}$ is the mean concentration (in mg/kg feed) during 5 days that can be found on crops or in insects, depending on the half-lifetime of the applied pesticide;
- The $\text{PEC}_{\text{feed,long}}$ is the mean concentration (in mg/kg feed) during a longer period (depending on the duration of the toxicity tests) that can be found on crops or in insects, depending on the half-lifetime of the applied pesticide.

The $\text{PEC}_{\text{feed,short}}$ and the $\text{PEC}_{\text{feed,long}}$ can be determined if the half-lifetime of the pesticides on crops or in insects can be calculated. The half-lifetime (DT_{50}) should preferably be determined from residue data on crops or insects. If 3 or more measured data are available, the DT_{50} can be determined by means of linear regression. If 2 measured data are available, the DT_{50} can be calculated as follows:

$$\text{DT}_{50} = \ln 2 * t / (\ln C_t - \ln C_0) \quad (\text{d})$$

in which: C_0 = concentration on feed at day = 0
 C_t = concentration on feed at day t
t = time

The mean concentration of a pesticide in feed during 5 or more days can be calculated as follows:

$$\text{PEC}_{\text{feed,short/long}} = C_0 * (1 - e^{-(k * t)}) / (k * t)$$

in which: $k = \ln 2 / \text{DT}_{50}$

Route 23. Uptake of soil (granules or treated seeds) by birds and mammals.

By eating granules or treated seeds from the soil, birds and mammals can be exposed to pesticides. The decision tree for these exposure routes is presented in Appendix 8 (Module B), and is developed after research by Luttik (1993). Input data of the decision tree are:

- $\text{LD}_{50_{\text{species of concern}}}$ (mg a.i./species of concern; see routes 21-22) R
- $\text{LD}_{50_{\text{granule}}}$ (granules) R
- Number of granules/treated seeds per square meter, corrected for the percentage mixed with the soil ($K; \text{m}^{-2}$; see routes 3 - 4) C

- PEC_{feed} (mg a.i./day) O
- Daily Feed Intake (g/day) C

The $LD50_{\text{granule}}$ is similar to the $LD50_{\text{target-group}}$ corrected for the amount of pesticide per granule/treated seed:

$$LD50_{\text{granule}} = LD50_{\text{target-group}} / \text{amount of pesticide per granule} \quad (\text{granule})$$

The PEC_{feed} can be defined as follows:

$$PEC_{\text{feed}} = Dos_{\text{sur}} * 10^6 / (H_{\text{soil}} * B_d) \quad (\text{For } Dos_{\text{sur}} \text{ see routes 1 \& 2})$$

Route 24. Uptake of water by birds and mammals.

Besides eating granules, treated seeds, crops or insects, birds and mammals can also be exposed to a pesticide by the uptake of water. This can be either surface water or water on leafs and crops. A decision tree for this exposure route is presented in Appendix 8 (Module D). It is based on research by Luttkik (1993). The decision tree has the following input data:

- $LD50_{\text{species of concern}}$ (mg a.i./species of concern) R
- $PEC_{\text{spray-liquid}}$ (mg a.i./l) O
- $PEC_{\text{wat, 0-5 days}}$ (mg a.i./l) O
- Daily Water Intake (g/day) C

The $PEC_{\text{spray-liquid}}$ can be determined as follows:

$$PEC_{\text{spray-liquid}} = \text{dosage (in kg a.i./ha)} / \text{amount of spray-liquid (in l/ha)}$$

It is assumed that birds with a mean body weight of maximum 100 g have a DWI of at most 30% of their bodyweight. For birds with a mean body weight higher than 100 g this is at most 10%. Biodegradation of the pesticide is not taken into consideration, unless it is very rapid ($DT50 < 1$ d).

The $PEC_{\text{wat, 0-5 days}}$ is determined by drift (route 6) and run-off/erosion (route 12):

$$PEC_{\text{wat, 0-5 days}} = PEC_{\text{short term}} + C_{\text{wat.r/e}}$$

Route 25. Exposure of and uptake by terrestrial organisms (e.g. earthworms) and effects on nitrification.

The decision tree for the exposure of terrestrial organisms is presented in Appendix 9. Input data of this decision tree are:

- Half life time for biodegradation (DT50; in days) R
- Lethal Concentration for 50% of the organisms (LC50; in mg a.i./kg) R
- NOEC (mg a.i./kg) R
- PIEC (mg a.i./kg) O (routes 1-4)
- Predicted Environmental Concentration in Soil (PEC; in mg a.i./kg)

For the Predicted Environmental Concentration in soil (PEC_{soil}) the mean concentration during a period of 4 weeks is taken. The method to calculate this concentration is shown in Table 26. An assumption is that degradation follows first order kinetics and is equal to the mean DT50 in the soil degradation studies.

Table 26. Model for calculation of mean concentration in soil after 4 weeks

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration at t_0 (mg a.i./kg)	$C_{soil,t=0}$ (or PIEC)	O
Half life time for biodegradation (d)	DT50	R
Time interval (d)	t	C
Output:		
Mean concentration during time interval (mg a.i./kg)	$C_{soil,mean}$ (or PEC)	
Model calculation:		
$C_{soil,mean} = C_0 * (1 - e^{-(k * t)}) / (k * t)$		
in which: $k = \ln 2 / DT50$		

Besides biodegradation, the concentration in the soil is also influenced by volatilization, uptake by organisms, and deposition. However, these processes are not (yet) taken into consideration.

The uptake of a pesticide by earthworms is calculated by means of the Bioconcentrationfactor (BCF) for soil - earthworm (Table 27). This BCF should preferably be derived experimentally. If no experimentally obtained data are available, it can be estimated by means of the following Quantitative Structure Activity Relationships (QSARs):

$$\text{BCF} = (0.01 / (0.66 * F_{oc})) * K_{ow}^{0.07}$$

in which: F_{oc} = fraction organic material

K_{ow} = Octanol-water partition coefficient

Table 27. Model for uptake by terrestrial organisms

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Bioconcentrationfactor for soil-earthworm	BCF	R/C
Predicted Environmental Concentration in soil (mg a.i./kg)	PEC	O
Output:		
Concentration in earthworms (mg a.i./kg)	C_{worm}	
Model calculation:		
$C_{worm} = \text{BCF} * \text{PEC}$		

The decision tree for the effects of pesticides on nitrification is presented in Appendix 10. It has the following input data:

- DT50 (d) R
- Effect concentration for 50% of the organisms (EC50; mg a.i./kg) R
- PIEC (mg a.i./kg) O (routes 1-4)

Route 26. Uptake of terrestrial organisms by birds and mammals.

The uptake of terrestrial organisms by birds and mammals, in other words, the secondary poisoning of birds and mammals, has been described by Romijn *et al.* (1991b). The from this research derived decision tree is presented in Appendix 8, module E. Only 3 parameters are used as input parameters:

- Bioconcentrationfactor (BCF) for soil - earthworm (mg a.i./kg) R/C
- NOEC for birds/mammals (mg a.i./kg) R
- $\text{PEC}_{\text{soil, 0-X days}}$ (mg a.i./kg) O (Table 26)

It has to be noticed that in the decision tree, corresponding to Romijn *et al.* (1991a), extrapolation methods are applied to derive a NOEC for birds or mammals.

Route 27. Exposure of and uptake by water organisms.

The decision tree for exposure of water organisms is presented in Appendix 11. This decision tree has the following input data:

- PEC_{wat, 0-4 days, 0-21 days, and 0-28 days} (mg a.i./l) O (route 6)
- LC50 for fish and crustaceans (mg a.i./l) R
- EC50 for algae (mg a.i./l) R
- NOEC for algae (4 days of exposure), crustaceans (21 days of exposure) and fish (28 days of exposure) (mg a.i./l) R

The concentration in water after 21 or 28 days is calculated in the same way as the concentration in soil after 28 days (see Table 26):

Table 28. Method for calculation of concentration in water after 21/28 days

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration at t_0 (mg a.i./kg)	$C_{\text{wat},0}^a$	O
Half life time for biodegradation (d)	DT50	R
Time interval (d)	$t = 21/28$	C
Output:		
Mean concentration during time interval (mg a.i./kg)	$C_{\text{wat},\text{mean}}$	

Model calculation:

$$C_{\text{wat},\text{mean}} = C_{\text{wat},0} * (1 - e^{-(k * t)}) / (k * t)$$

$$\text{in which: } k = \ln 2 / \text{DT50}$$

^a Calculated with SLOOT.BOX

Although drainage (route 14) is a long term, chronic process, it might be added to the process of drift, giving the following water concentration after 21 or 28 days:

$$C_{\text{wat}} = C_{\text{wat},\text{mean}} + C_{\text{wat},\text{drai}} \quad (\text{mg a.i./l})$$

The uptake of pesticides by water organisms is calculated by means of the Bioconcentrationfactor (BCF). If no experimentally derived BCF is available, the following QSAR-calculation can be used:

$$BCF = 0.048 * K_{ow}$$

in which: K_{ow} = Octanol-water partition coefficient

The model for calculating the concentration of the pesticide in water organisms is presented in Table 29.

Table 29. Model for uptake by water organisms

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Bioconcentrationfactor water - water organism (-)	BCF	R/C
Predicted Environmental Concentration (mg a.i./l)	PEC _{wat}	O
Output:		
Concentration in water organism (mg a.i./kg)	C _{wat.org}	
Model calculation:		
$C_{wat.org} = BCF * PEC_{wat}$		

Route 28. Uptake of water organisms by birds and mammals.

Uptake of water organisms by birds and mammals (secondary poisoning) has been described by Romijn *et al.* (1991a). The corresponding decision trees is presented in Appendix 8 (Module E). It has the following input data:

- PEC_{wat,0-X days} (mg a.i./l) O (route 6)
- BCF (mg a.i./kg) R
- NOEC for birds and mammals (mg a.i./l) R

According to Romijn *et al.* (1991a), in the decision tree extrapolation methods are used to derive a NOEC for birds or mammals.

Route 29. Consumption of crops by man.

The consumption of crops by man, the PlantDose, is a part of the Total Daily Intake module, described by Toet *et al.* (1991). It is assumed that the uptake of pesticides in the plants via leaf is negligible, as well as the concentration left on the leaf when harvested. Therefore, the dosage of a pesticide taken up by man via plants is only dependent on the concentration in

crops as a result of uptake from the soil (route 19). The model for crop-consumption is described in Table 30.

Table 30. Model for consumption of crops by man

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration in plants (mg a.i./kg w.w.)	C_{plant}	O (route 19)
Daily intake of crops (kg/d)	PlantInt	C
Average human body weight (kg)	BW	C
Output:		
Total Plant Dose (mg/kg bw/d)	Dos_{plant}	
Model calculation:		
$Dos_{\text{plant}} = C_{\text{plant}} * \text{PlantInt} / \text{BW}$		

Route 30. Consumption of fish by man.

The consumption of fish by man is a part of the Total Daily Intake module described by Toet *et al.* (1991) and Van de Meent & Toet (1992). The fish module is described in Table 31.

Table 31. Model for consumption of fish by man

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
(Dissolved) surface water concentration (mg a.i./l)	$C_{\text{wat(.dis)}}$	O (routes 8 and 27)
Octanol/water partition coefficient (-)	K_{ow}	R
Daily intake of fish (kg/d)	FishInt	C
Average human body weight (kg)	BW	C
Output:		
Bioconcentration factor (l/kg)	BCF_{fish}	
Concentration in fish (mg/kg)	C_{fish}	
Total fish dose (mg/kg bw/d)	FishDose	

(to be continued)

Table 30. (continued)**Model Calculations:***Bioconcentration factor*

$$BCF_{fish} = 0.05 * K_{ow}$$

Concentration in fish

$$C_{fish} = BCF_{fish} * C_{wat.dis}$$

Total fish dose

$$FishDose = C_{fish} * FishInt / BW$$

Route 31. Consumption of meat and milk by man.

The consumption of meat and milk by man is described in the cattle module of Toet *et al.* (1991). According to Travis & Arms (1988), consumption can be modelled by means of biotransfer factors, defined as the steady state concentration in a receiving medium (meat, milk; mg/kg wwt) divided by the animals' daily contaminant intake (mg/d). A bioconcentration factor can be calculated from the daily intake of source media: grass and soil. Intake through air by cattle is neglected as well as differences in grass and soil intake between lactating and non-lactating cattle.

Table 32. Consumption of meat and milk by man

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration in grass (mg a.i./kg)	C_{grass}	O (route 19)
Concentration in grassland soil (mg a.i./kg)	$C_{soil.g}$	O (table 26)
Octanol/water partition coefficient (-)	K_{ow}	R
Daily uptake of grass (kg dwt/d)	$Grass_{Upt}$	C
Daily uptake of soil (kg dwt/d)	$Soil_{Upt}$	C
Conversion fresh to dry weight plants (-)	$Conv_{pl}$	C
Conversion total to dry soil concentration (-)	$Conv_{soil}$	C
Daily intake of milk (kg/d)	$MilkInt$	C
Daily intake of beef (kg/d)	$BeefInt$	C
Average human bodyweight (kg)	BW	C

(to be continued)

Table 32. (continued)

Parameter/variable (unit)	Symbol	C/R/E/O
Output:		
Biotransfer factor for cows (-)	BTF_{cow}	
Biotransfer factor for milk (-)	BTF_{milk}	
Concentration in beef (mg/kg wwt)	C_{beef}	
Concentration in milk (mg/kg wwt)	C_{milk}	
Total milk dose (mg/kg bw/d)	MilkDose	
Total beef dose (mg/kg bw/d)	BeefDose	

Model calculations:*Biotransfer factors*

$$BTF_{cow} = 10^{-7.6 + \log Kow}$$

$$BTF_{milk} = 10^{-8.1 + \log Kow}$$

Uptake of pesticides

$$C_{beef} = BTF_{cow} * (C_{grass} * GrassUpt * Conv_{pl} + C_{soil.g} * SoilUpt * Conv_{soil})$$

$$C_{milk} = BTF_{milk} * (C_{grass} * GrassUpt * Conv_{pl} + C_{soil.g} * SoilUpt * Conv_{soil})$$

Milk and beef dose

$$MilkDose = C_{milk} * MilkInt / BW$$

$$BeefDose = C_{beef} * BeefInt / BW$$

Route 32. Intake of drinking water by man.

The model for the daily intake of drinking water by man, together with other exposition sources, has been described by Toet *et al.* (1991). It is presented in Table 33.

Table 33. Module for daily intake of drinking water

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration in drinking water (mg/l)	$C_{dr.wat}$	O (routes 16 and 17)
Average human body weight (kg)	BW	C
Daily intake of drinking water (l/d)	DrinkInt	C
Output:		
Daily dose via drinking water (mg/kg BW/d)	DrinkDose	
Model calculation:		
$DrinkDose = DrinkInt * C_{dr.wat} / BW$		

Route 33. Inhalation of air by man.

For the calculation of the inhalation of air by man, the concentration in air at a distance of 100 m from the source ($\mu\text{g}/\text{m}^3$; see route 5) is used. It is assumed that the inhalation rate for man is $0.83 \text{ m}^3/\text{h}$ (or $20 \text{ m}^3/\text{d}$). The inhalation model can be described with the following model:

Table 34. Model for calculating oral intakes after inhalation

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Concentration in air (100 m from source; $\mu\text{g}/\text{m}^3$)	C_{air}	O (route 5)
Inhalation rate (m^3/h)	$IR = 0.83$	C
Time of exposure per day (h)	t_{exp}	E
Inhalation bio-availability	$B_{ihl} = 0.75$	C
Body weight humans (kg)	BW	C
Oral bio-availability	$B_{oral} = 1$	C
Output:		
Oral intake after inhalation (mg/kg bw/day)	I_{orl}	
Model calculation:		
$I_{orl} = C_{air} * IR * t * B_{ihl} / (BW * B_{oral})$		

The uptake of pesticides by man via the various sources, the Total Human Dose (in mg/kg bw/d) can now be described as follows:

$$\text{TotHumanDose} = \text{DrinkDose} + \text{FishDose} + \text{PlantDose} + \text{MilkDose} + \text{BeefDose} + I_{\text{ort}}$$

In the hazard assessment model for human beings, this total daily intake by human beings is compared to the No Observed Adverse Effect Level (NOAEL). The result is a Margin of Safety for human beings (Table 35) (Toet *et al.* 1991).

Table 35. Hazard assessment for human beings

Parameter/variable (unit)	Symbol	C/R/E/O
Input:		
Total daily intake by human beings (mg/kg bw/d)	TotHumanDose	O
No Observed Adverse Effect Level for mammals (rat) (mg/kg bw)	NOAEL	R
Output:		
Margin of safety for human beings (-)	Human hazard	

Model calculation:

$$\text{HumanHazard} = \text{NOAEL} / \text{TotHumanDose}$$

4. CONCLUSIONS AND RECOMMENDATIONS

This report presents the first detailed overview of the evaluation or risk assessment system for agricultural pesticides, as a part of the Evaluation System for Pesticides (ESPE). This risk assessment system involves the integration of exposure and effects data. The system does not yet involve uncertainty analysis. This uncertainty arises from variability in the environment and in human conduct, and from limitations in model descriptions and data used. The integration of the data does not cover every possible exposure and effect route, but the knowledge and expert judgement of the, at this moment, most relevant routes are taken into consideration.

The evaluation system for agricultural pesticides presents good starting points for integration in the USES project. Where possible, the same route descriptions as in DRANC and PRISEC are used. Other route descriptions, specific for this risk assessment system, are possibly useful for DRANC and PRISEC. However, before publication of the first version of USES in late 1993, several improvements of the evaluation system for agricultural pesticides should be introduced:

- * The system should be geared for integration into USES and should be further harmonized with the other USES sub-systems, namely DRANC and PRISEC. In addition, the evaluation system for non-agricultural pesticides, which will be published in 1993, should also be incorporated into USES.
- * As applied in the decision trees for birds and mammals, extrapolation methods can be used to derive a NOEC for a group of organisms instead of using the lowest NOEC per group of organisms (Romijn *et al.*, 1991a). Therefore, extrapolation methods should be incorporated in all other decision trees as soon as a method accepted by the OECD is available.
- * An uncertainty and variance analysis should be developed for this system.

Recommendations for further research and developments, but with less priority, are:

- * The assessment system model for pesticides should be validated. The usefulness of e.g. the OPS model, used for the calculation of the concentration of a substance at a distance of 100 m from diffuse sources instead of a point source, should be proved. Routes like volatilization from soil, water and crops can be conceived as diffuse sources, while the OPS-model assumes point sources. In this validation, the relevance of some routes, like atmospheric deposition, should also be determined.
In future, a comparison of calculated values with measured values should be performed where possible.
- * Some exposure or effect routes, now considered as negligible or not yet taken into account, should be elaborated. One of these routes is foliar uptake of chemicals by plants. It increasingly appears that uptake of chemicals by vegetation is a major source of food chain bioaccumulation and an important route of exposure to humans and animals (Paterson *et al.*, 1990). Literature research has shown that the pathway of foliar uptake may contribute

more to the total plant residues than root uptake (Topp *et al.*, 1986). Two processes precede the penetration of chemicals, present in soil, into leaf tissues via the air:

1. volatilization from soil;
2. deposition from the air onto leaf surfaces.

The uptake via vapour in the air is related both to the volatility of the chemical from the soil and to the deposition velocity of chemical vapour from the air to plant surfaces. Paterson *et al.* (1991) described a three compartment (root, stem and leaf) model of a plant in which chemical uptake from soil and/or air is quantified.

Other routes or aspects which should be elaborated are e.g.

- exposure of insects, birds and mammals via air;
 - exposure of (non target) plants;
 - accounting residue-data on crops at calculation human consumption of crops;
 - percolation of surface water and well formation in the soil.
- * A comparison of calculated concentrations in plant material with residue levels as established by the Joint Meeting on Pesticides Residues (JMPR) of the WHO/FAO should be carried out.
- * An estimation procedure for hazards of pesticides and pesticide leachates to sediment and groundwater organisms should be developed.
- * Some parameters, particularly the percentages of interception by crops, should be extended or adjusted. At the moment, the part of the dosage that reaches the soil or is intercepted by the crop is supposed to be 90%, leaving 10% for air-emission. This value should be supported by literature research. Also an extension of the number of crops (at this moment seven kinds) should be taken into consideration.
- * Other application possibilities, like application as aerosols, seed disinfectants in silos, or evaporation substances, should be incorporated in the system.

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Appendix 2: PESTLA-calculations for determining concentrations in groundwater, percentage of leaching and amount of pesticide in plough layer

- DT50 : Halflife time (d)
 KOM : Sorption factor, based on organic matter content (l/kg)
 C_dmax : Maximal conc. deeper groundwater (ug/l)
 %PER : Percentage of dosage leached below a depth of 1 m.
 %ACC : Percentage of dosage still present in top soil (0-0.2 m), after a period of 1 year

Note: all data based on a single application dose of 1 kg/ha, in the springtime.

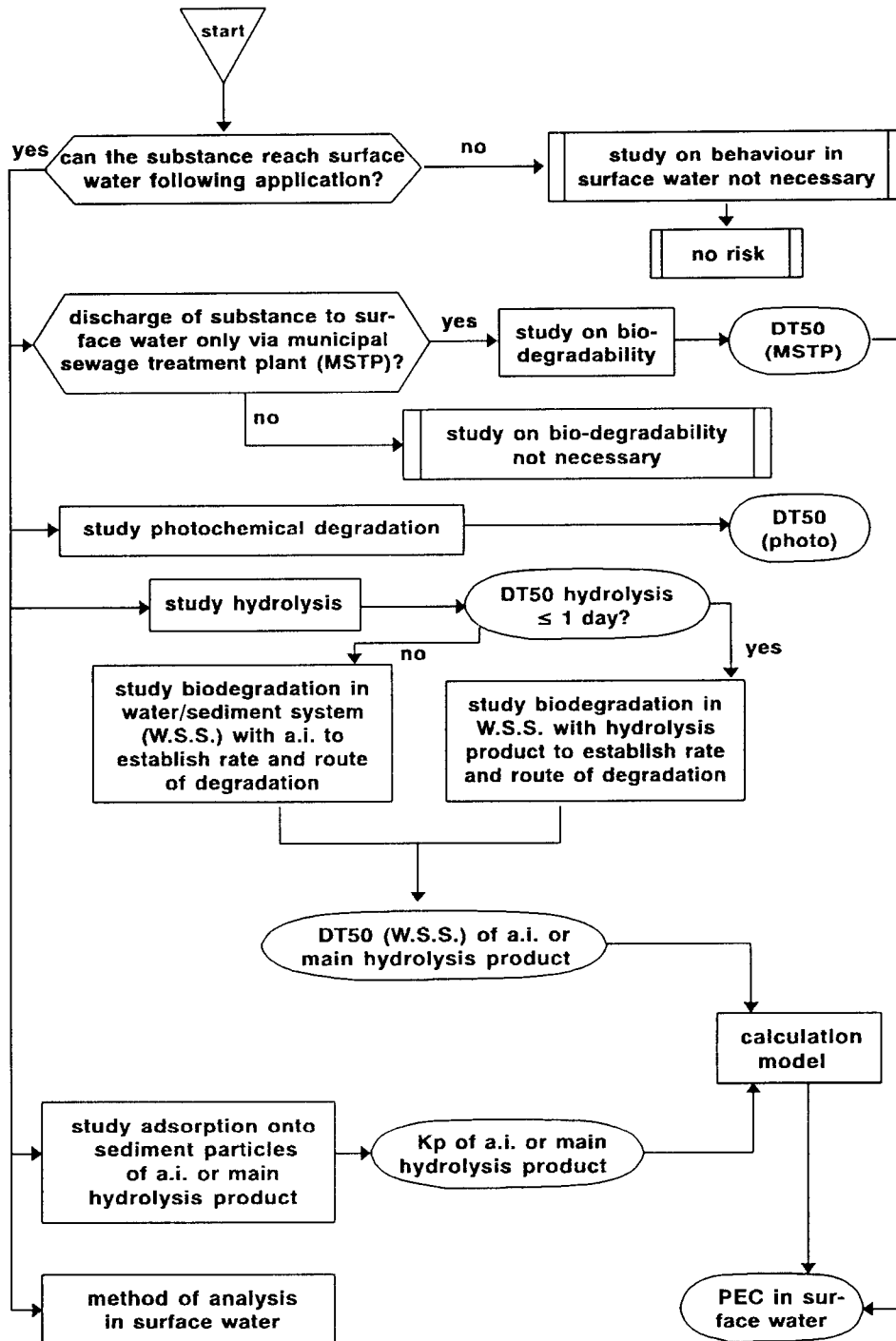
DT50	KOM	C _d max	%PER	%ACC
0.0	0.0	0.0000	0.000	0.000
5.0	0.0	0.0225	0.003	0.000
10.0	0.0	0.3100	0.120	0.000
20.0	0.0	3.1900	1.270	0.000
40.0	0.0	14.2000	5.710	0.000
60.0	0.0	24.4000	9.880	0.000
80.0	0.0	32.3000	13.100	0.000
100.0	0.0	38.3000	15.600	0.000
150.0	0.0	48.2000	19.600	0.000
200.0	0.0	54.1000	22.100	0.000
300.0	0.0	60.8000	24.814	0.001
400.0	0.0	64.4600	26.332	0.001
500.0	0.0	66.7700	27.240	0.001
0.0	10.0	0.0000	0.000	0.000
5.0	10.0	0.0000	0.000	0.000
10.0	10.0	0.0073	0.003	0.000
20.0	10.0	0.8056	0.320	0.000
40.0	10.0	8.9600	3.870	0.170
60.0	10.0	20.3800	9.140	0.440
80.0	10.0	30.8000	14.210	0.700
100.0	10.0	39.4900	18.630	0.930
150.0	10.0	55.0300	26.930	1.350
200.0	10.0	64.9600	32.510	1.620
300.0	10.0	76.7100	39.390	1.950
400.0	10.0	83.3500	43.412	2.150
500.0	10.0	87.6100	46.042	2.270
0.0	20.0	0.0000	0.000	0.000
5.0	20.0	0.0000	0.000	0.000

DT50	KOM	C _d max	%PER	%ACC
10.0	20.0	0.0006	0.000	0.000
20.0	20.0	0.2137	0.082	0.035
40.0	20.0	3.9800	1.750	0.680
60.0	20.0	10.4600	5.225	1.830
80.0	20.0	16.9600	9.310	2.980
100.0	20.0	22.9210	13.370	4.000
150.0	20.0	35.6600	22.180	5.920
200.0	20.0	44.8000	28.900	7.200
300.0	20.0	56.7500	38.085	8.760
400.0	20.0	64.0300	43.903	9.650
500.0	20.0	68.9200	47.888	10.240
0.0	40.0	0.0000	0.000	0.000
5.0	40.0	0.0000	0.000	0.000
10.0	40.0	0.0000	0.000	0.000
20.0	40.0	0.0067	0.003	0.008
40.0	40.0	0.3700	0.210	1.770
60.0	40.0	1.6700	1.090	4.960
80.0	40.0	3.8700	2.670	8.290
100.0	40.0	6.5400	4.720	11.270
150.0	40.0	13.6000	10.630	16.980
200.0	40.0	19.8000	16.440	20.800
300.0	40.0	29.0010	26.055	25.550
400.0	40.0	35.0900	33.182	28.300
500.0	40.0	39.3400	38.523	30.080
0.0	60.0	0.0000	0.000	0.000
5.0	60.0	0.0000	0.000	0.000
10.0	60.0	0.0000	0.000	0.000
20.0	60.0	0.0001	0.000	0.100
40.0	60.0	0.0410	0.025	2.510
60.0	60.0	0.3460	0.230	7.220
80.0	60.0	1.0200	0.780	12.220
100.0	60.0	2.0100	1.680	16.750
150.0	60.0	5.3100	5.060	25.500
200.0	60.0	8.8900	9.150	31.400
300.0	60.0	15.2300	17.171	38.760
400.0	60.0	20.1110	23.970	43.030
500.0	60.0	23.7500	29.476	45.820
0.0	80.0	0.0000	0.000	0.000
5.0	80.0	0.0000	0.000	0.000
10.0	80.0	0.0000	0.000	0.000
20.0	80.0	0.0000	0.000	0.116
40.0	80.0	0.0053	0.003	2.950

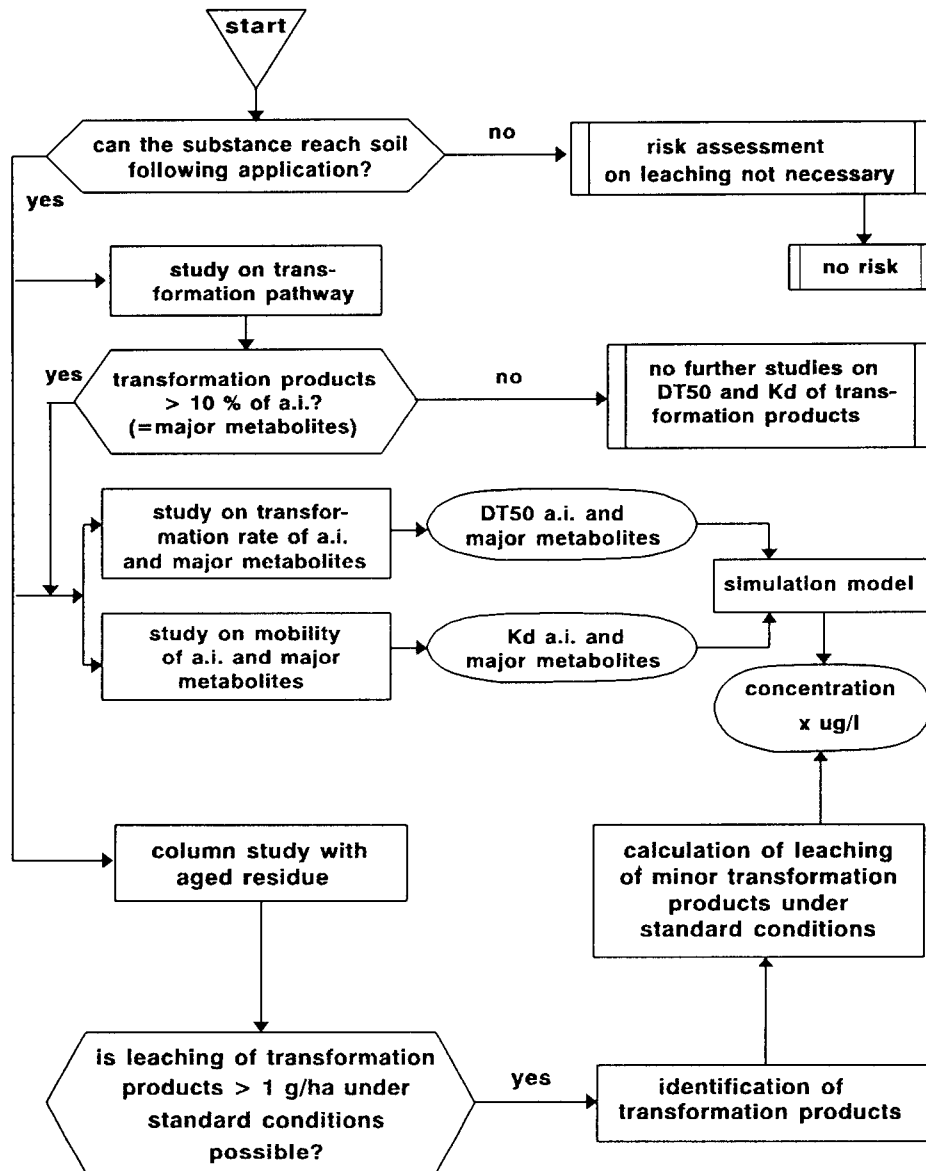
DT50	KOM	C _d max	%PER	%ACC
60.0	80.0	0.0700	0.055	8.610
80.0	80.0	0.2800	0.240	14.700
100.0	80.0	0.6800	0.630	20.200
150.0	80.0	2.3500	2.470	31.000
200.0	80.0	4.4100	5.170	38.400
300.0	80.0	8.4800	11.304	47.500
400.0	80.0	12.0330	17.140	52.830
500.0	80.0	14.9300	22.189	56.310
0.0	100.0	0.0000	0.000	0.000
5.0	100.0	0.0000	0.000	0.000
10.0	100.0	0.0000	0.000	0.000
20.0	100.0	0.0000	0.000	0.120
40.0	100.0	0.0007	0.000	3.190
60.0	100.0	0.0163	0.013	9.420
80.0	100.0	0.0877	0.079	16.180
100.0	100.0	0.2434	0.245	22.370
150.0	100.0	1.0245	1.230	34.440
200.0	100.0	2.2330	2.960	42.700
300.0	100.0	5.0500	7.434	52.990
400.0	100.0	7.6800	12.148	59.010
500.0	100.0	9.8700	16.466	62.950
0.0	150.0	0.0000	0.000	0.000
5.0	150.0	0.0000	0.000	0.000
10.0	150.0	0.0000	0.000	0.000
20.0	150.0	0.0000	0.000	0.126
40.0	150.0	0.0000	0.000	3.430
60.0	150.0	0.0005	0.001	10.300
80.0	150.0	0.0049	0.005	17.800
100.0	150.0	0.0210	0.025	24.700
150.0	150.0	0.1600	0.232	38.300
200.0	150.0	0.4800	0.775	47.700
300.0	150.0	1.4800	2.580	59.340
400.0	150.0	2.7140	4.941	66.190
500.0	150.0	3.9500	7.365	70.680
0.0	200.0	0.0000	0.000	0.000
5.0	200.0	0.0000	0.000	0.000
10.0	200.0	0.0000	0.000	0.000
20.0	200.0	0.0000	0.000	0.126
40.0	200.0	0.0000	0.000	3.490
60.0	200.0	0.0000	0.000	10.540
80.0	200.0	0.0003	0.000	18.290
100.0	200.0	0.0021	0.003	25.470

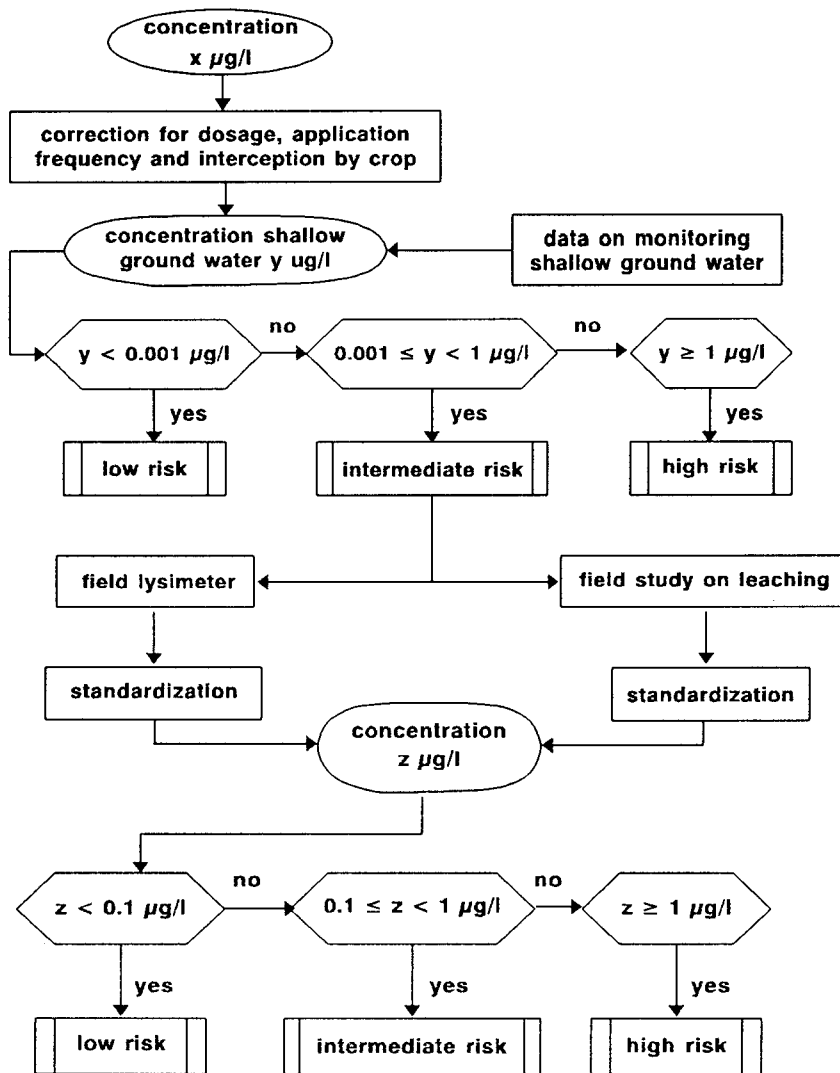
DT50	KOM	C_d max	%PER	%ACC
150.0	200.0	0.0285	0.047	39.600
200.0	200.0	0.1153	0.216	49.300
300.0	200.0	0.5000	0.863	61.510
400.0	200.0	1.0840	1.882	68.670
500.0	200.0	1.7400	3.026	73.360
0.0	300.0	0.0000	0.000	0.000
5.0	300.0	0.0000	0.000	0.000
10.0	300.0	0.0000	0.000	0.000
20.0	300.0	0.0000	0.000	0.130
40.0	300.0	0.0000	0.000	3.520
60.0	300.0	0.0000	0.000	10.670
80.0	300.0	0.0000	0.000	18.600
100.0	300.0	0.0000	0.000	25.900
150.0	300.0	0.0011	0.002	40.340
200.0	300.0	0.0081	0.011	50.350
300.0	300.0	0.0672	0.081	62.840
400.0	300.0	100.0	0.218	70.200
500.0	300.0	100.0	0.397	75.020
0.0	400.0	0.0000	0.000	0.000
5.0	400.0	0.0000	0.000	0.000
10.0	400.0	0.0000	0.000	0.000
20.0	400.0	0.0000	0.000	0.130
40.0	400.0	0.0000	0.000	3.520
60.0	400.0	0.0000	0.000	10.700
80.0	400.0	0.0000	0.000	18.640
100.0	400.0	0.0000	0.000	26.010
150.0	400.0	0.0000	0.000	40.560
200.0	400.0	100.0	0.001	50.645
300.0	400.0	100.0	0.006	63.240
400.0	400.0	100.0	0.019	70.660
500.0	400.0	100.0	0.200	75.530
0.0	500.0	0.0000	0.000	0.000
5.0	500.0	0.0000	0.000	0.000
10.0	500.0	0.0000	0.000	0.001
20.0	500.0	0.0000	0.000	0.120
40.0	500.0	0.0000	0.000	3.520
60.0	500.0	0.0000	0.000	10.710
80.0	500.0	0.0000	0.000	18.670
100.0	500.0	0.0000	0.000	26.060
150.0	500.0	100.0	0.000	40.660
200.0	500.0	100.0	0.000	50.780
300.0	500.0	100.0	0.000	63.420
400.0	500.0	100.0	0.001	70.880
500.0	500.0	100.0	0.010	75.770

Appendix 3: Decision tree for behaviour in water

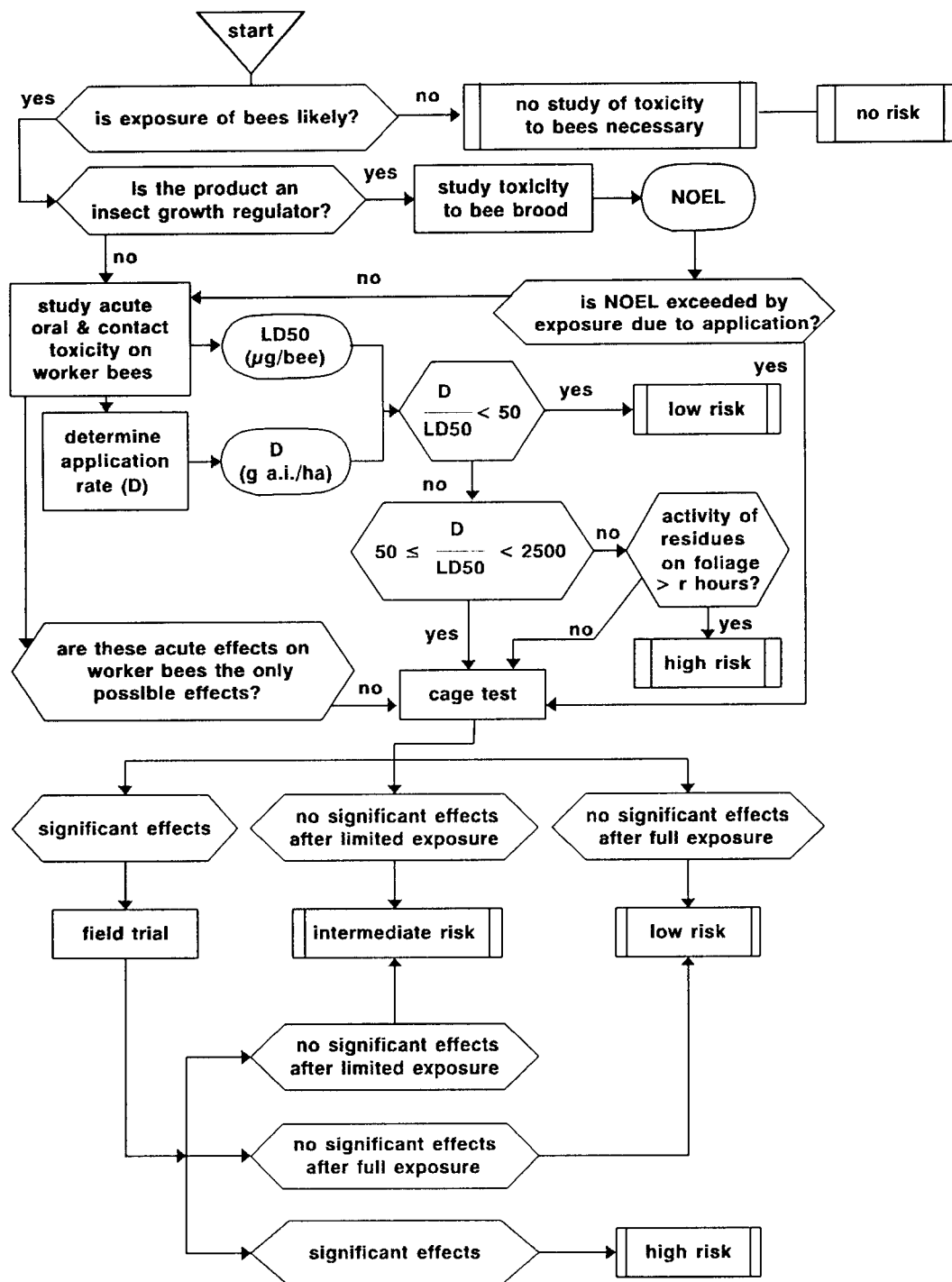


Appendix 4: Decision tree for leaching to shallow groundwater

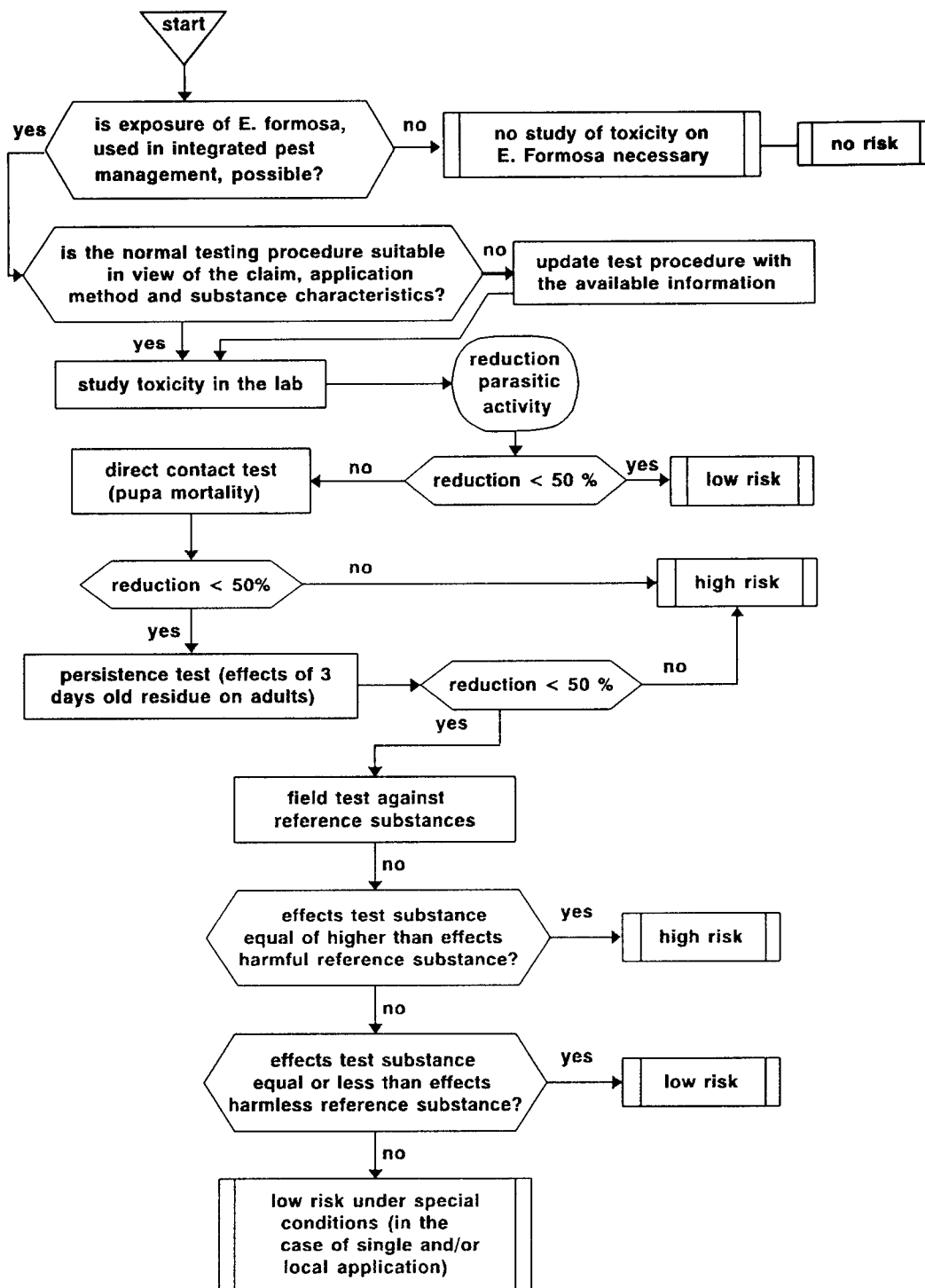


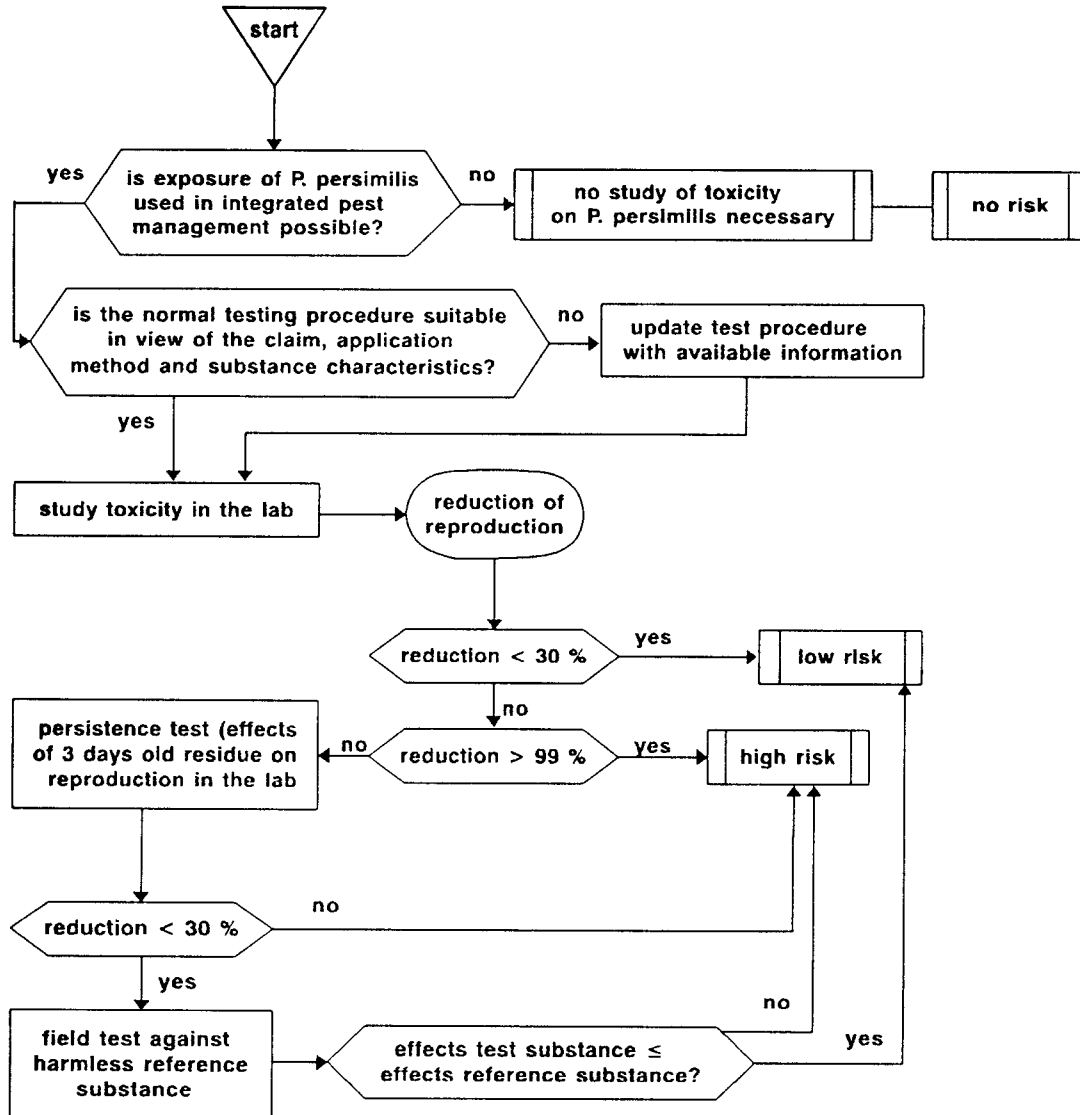


Appendix 5: Decision tree for bees



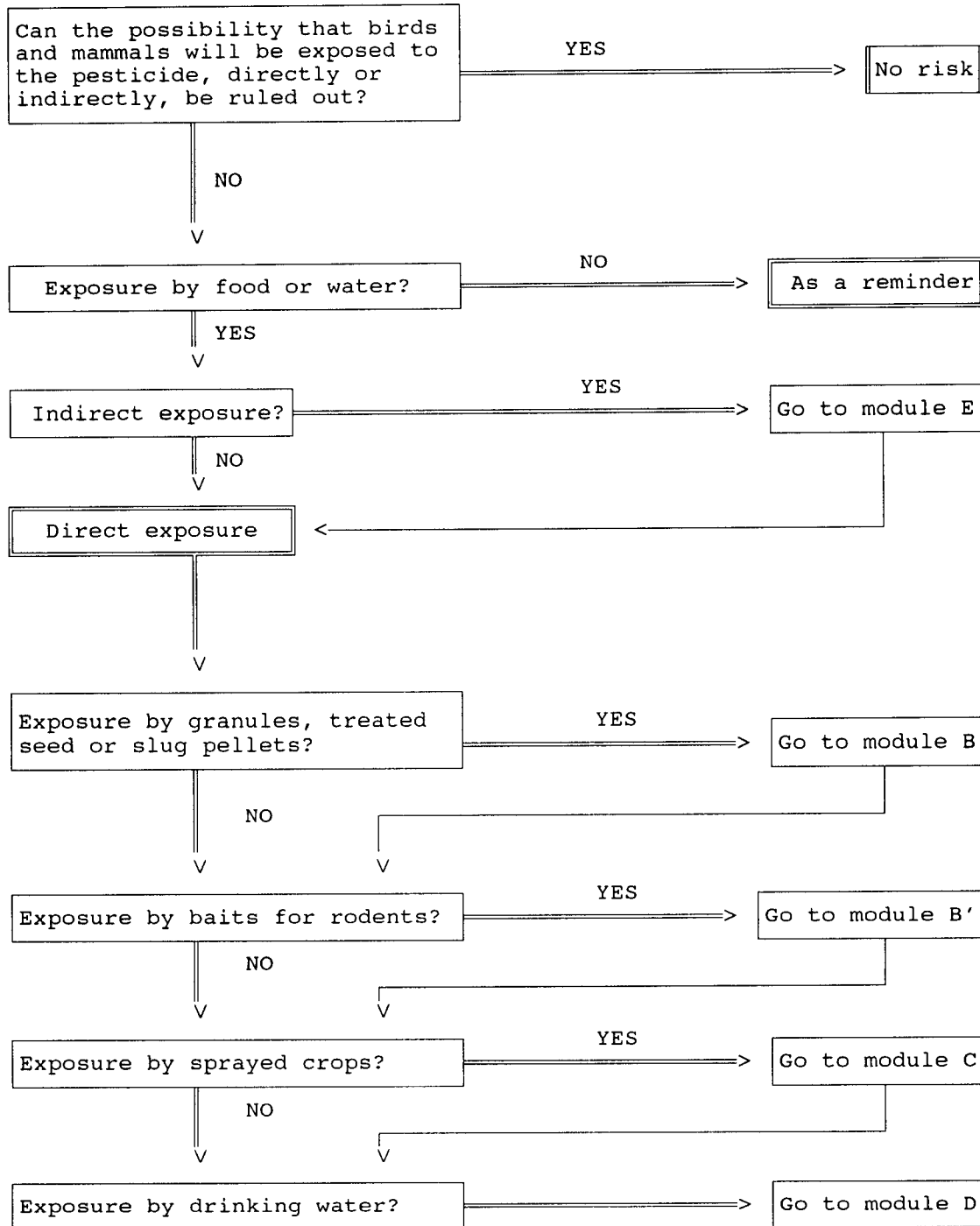
Appendix 6: Decision tree for *Encarsia formosa*



Appendix 7: Decision tree for *Phytoseiulus persimilis*

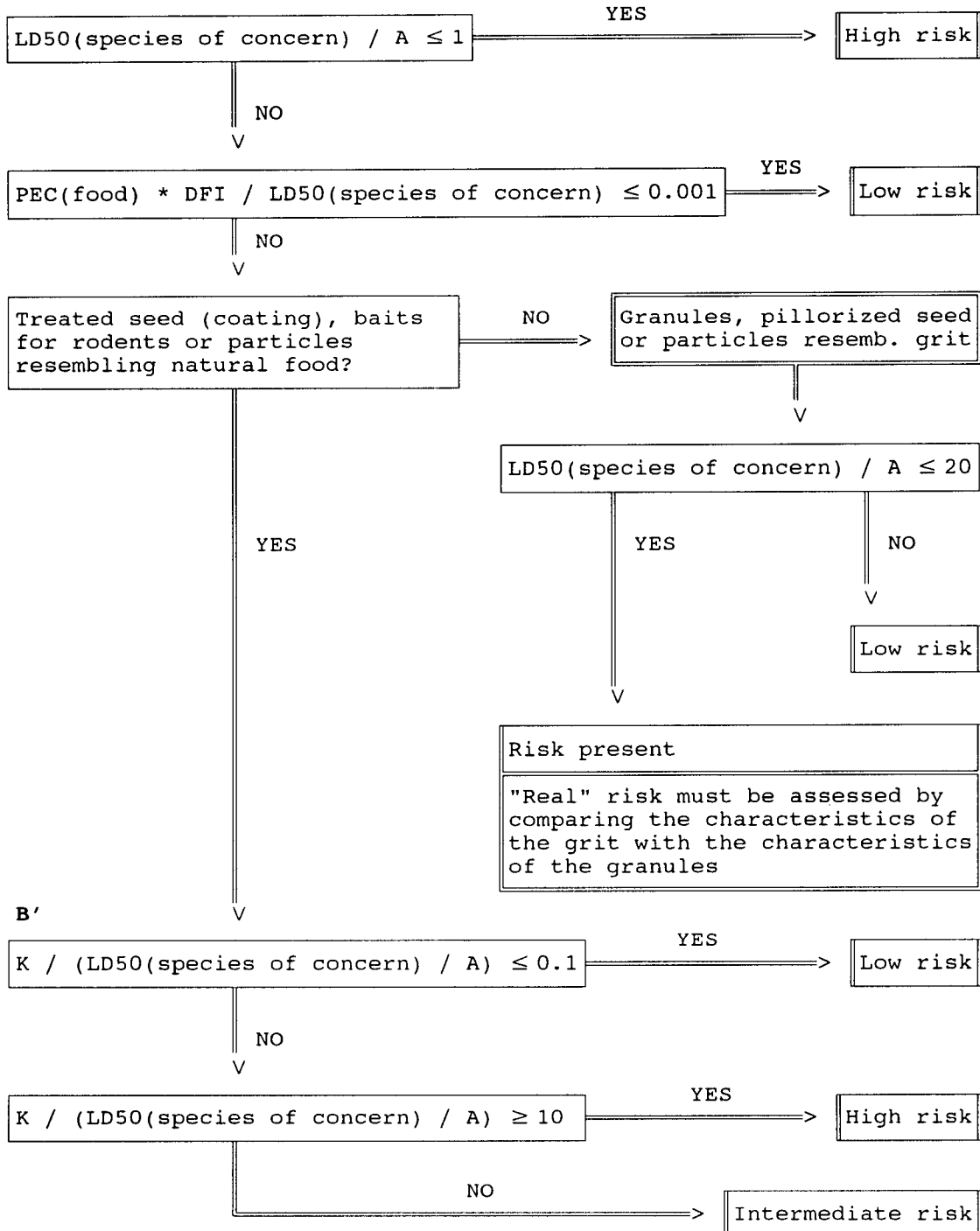
Appendix 8: Decision tree for birds and mammals

MODULE A General module for birds as well as mammals



MODULE B AND B' Exposure by granules, treated seed (including pillorized seed), baits for snails (starting at B) and baits for rodents (starting at B') for birds.

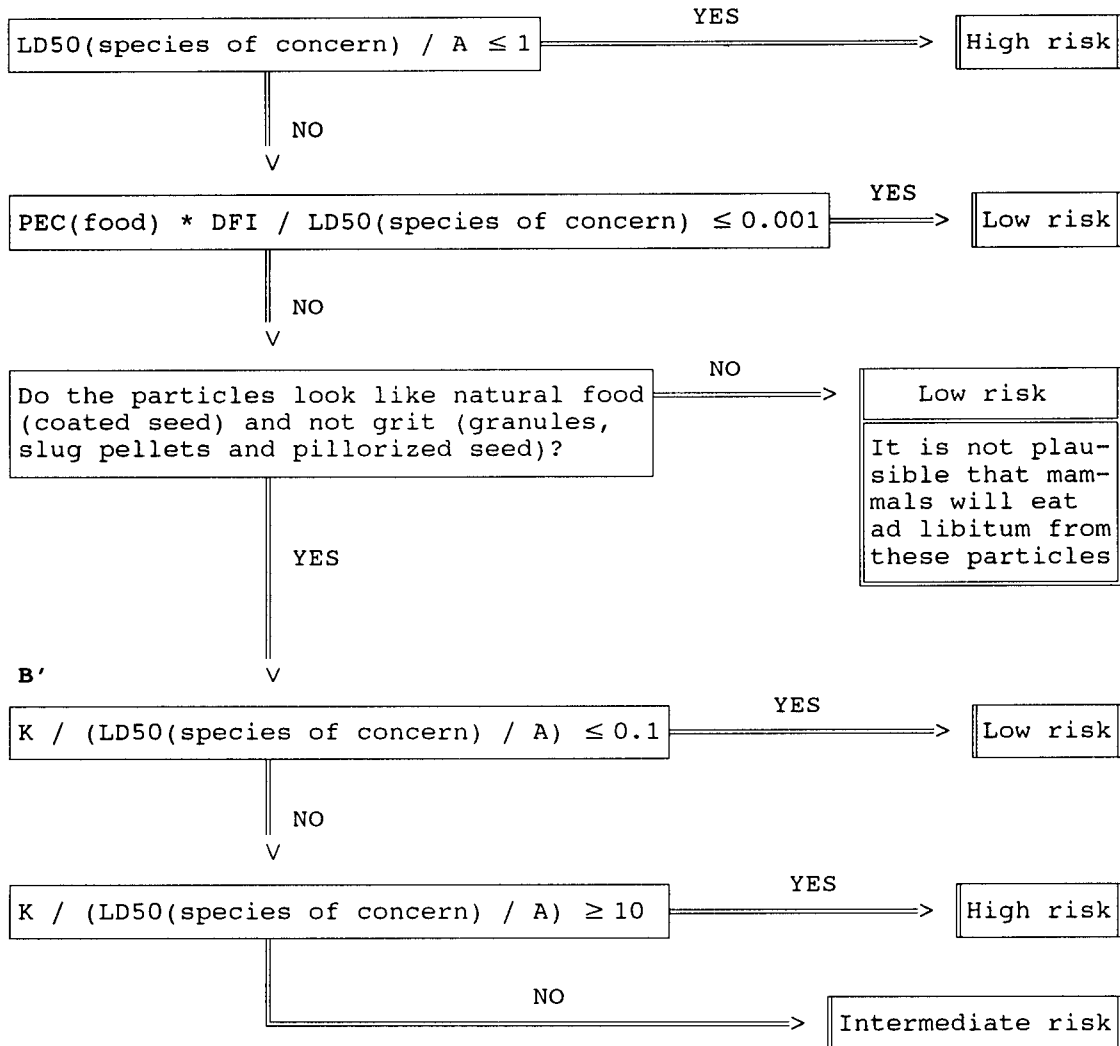
B



B'

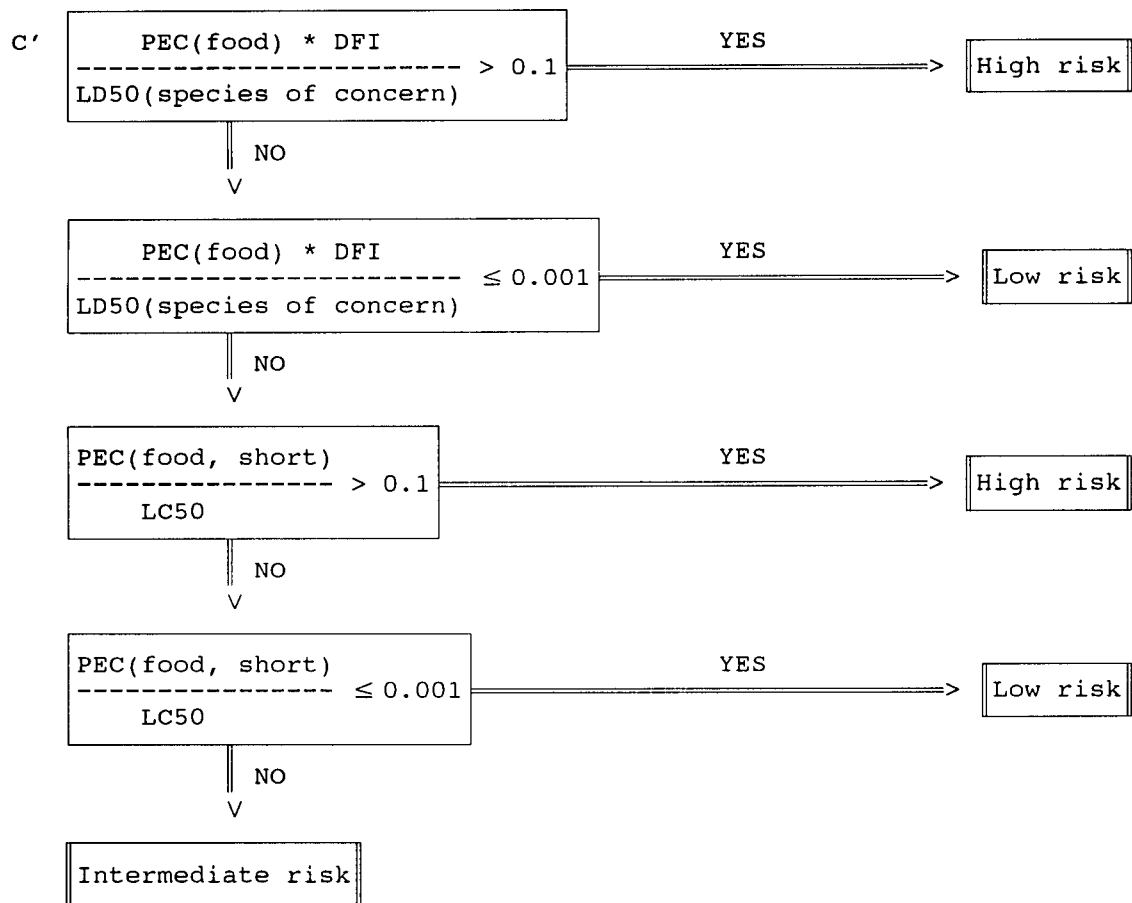
MODULE B AND B' Exposure by granules, treated seed (including pillorized seed), baits for snails (starting at B) and baits for rodents (starting at B') for mammals.

B

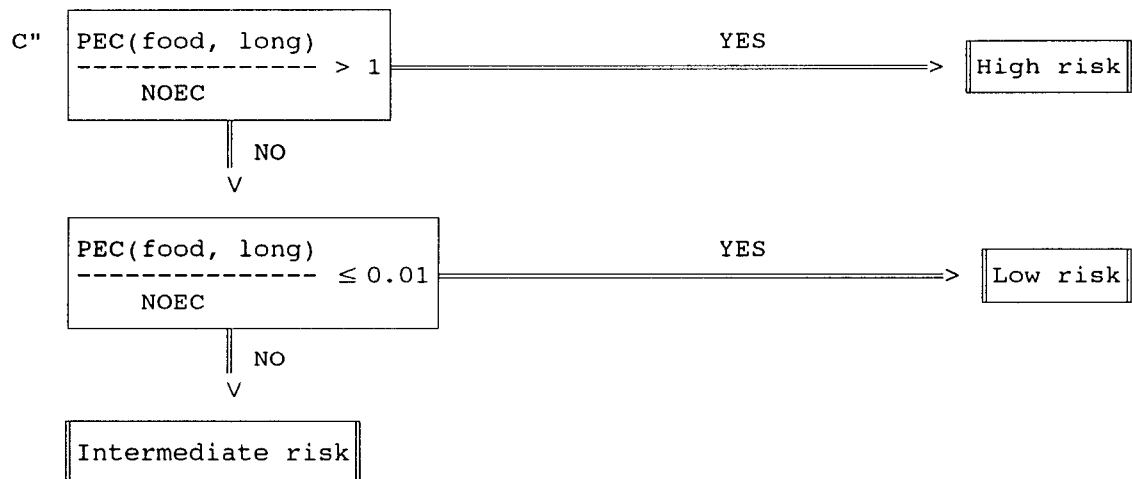


MODULE C Exposure by pesticides used for spraying crops/plants (insects) for birds. The risk for short term exposure can be assessed with part C' and long term exposure with part C".

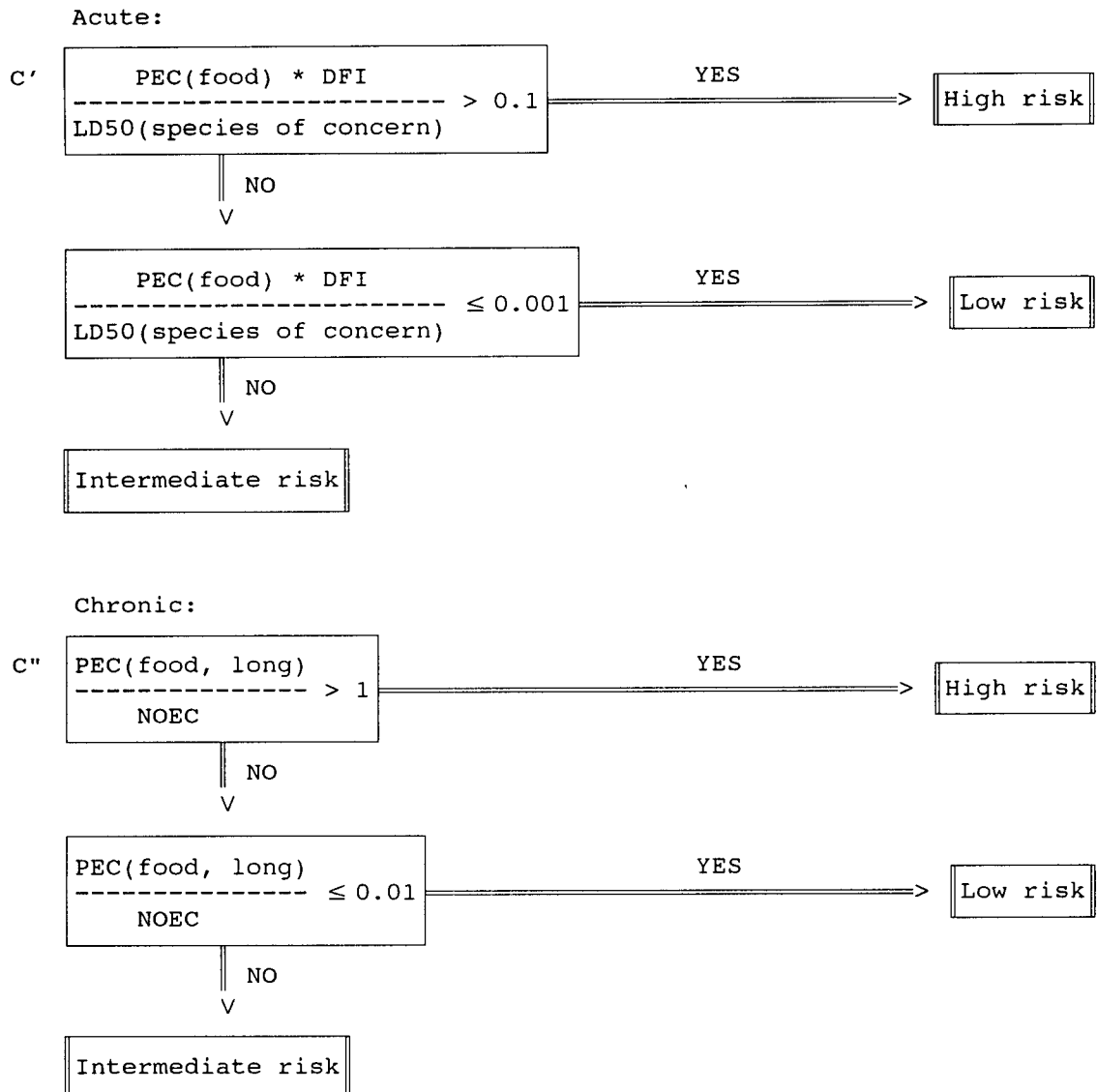
Acute:



Chronic:

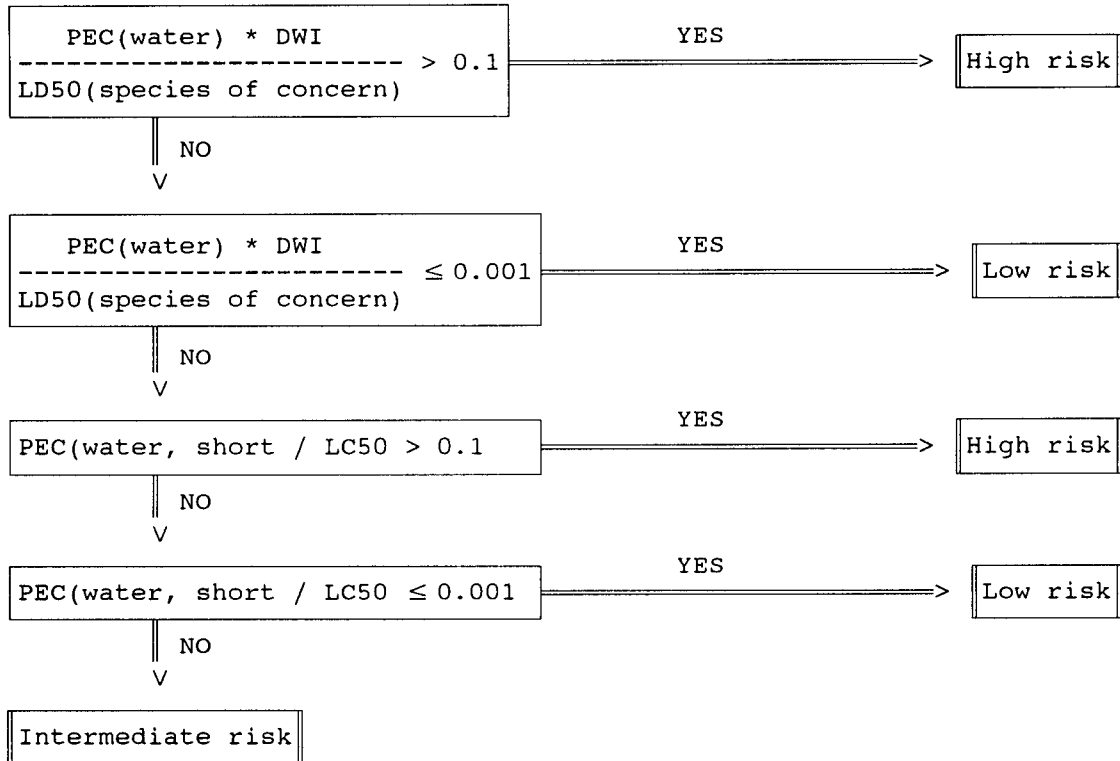


MODULE C Exposure by pesticides used for spraying crops/plants (insects) for mammals. The risk for short term exposure can be assessed with part C' and long term exposure with part C".

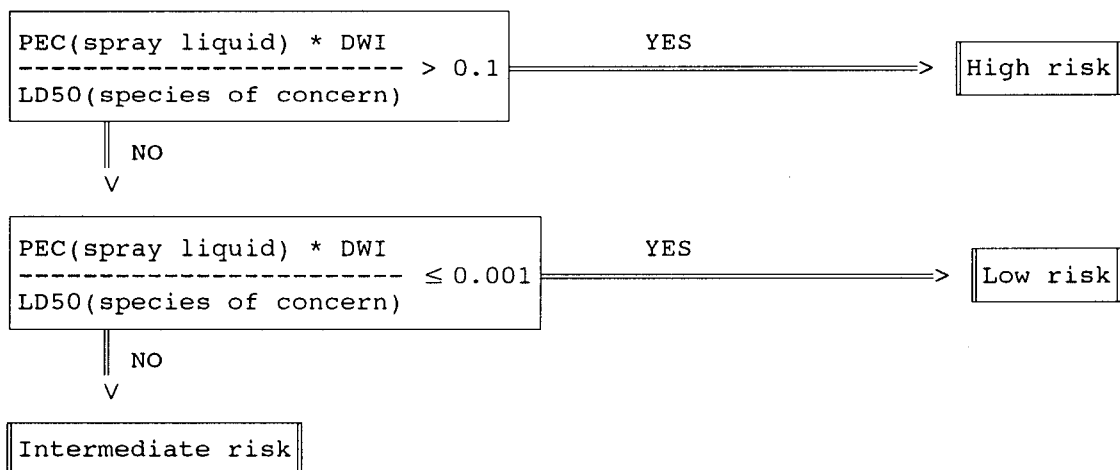


MODULE D Exposure by (drinking)water for birds. The risk for exposure by drinking water from surface water can be assessed with part D' and the risk for exposure by spray liquid in puddles or axis of leaves with part D"

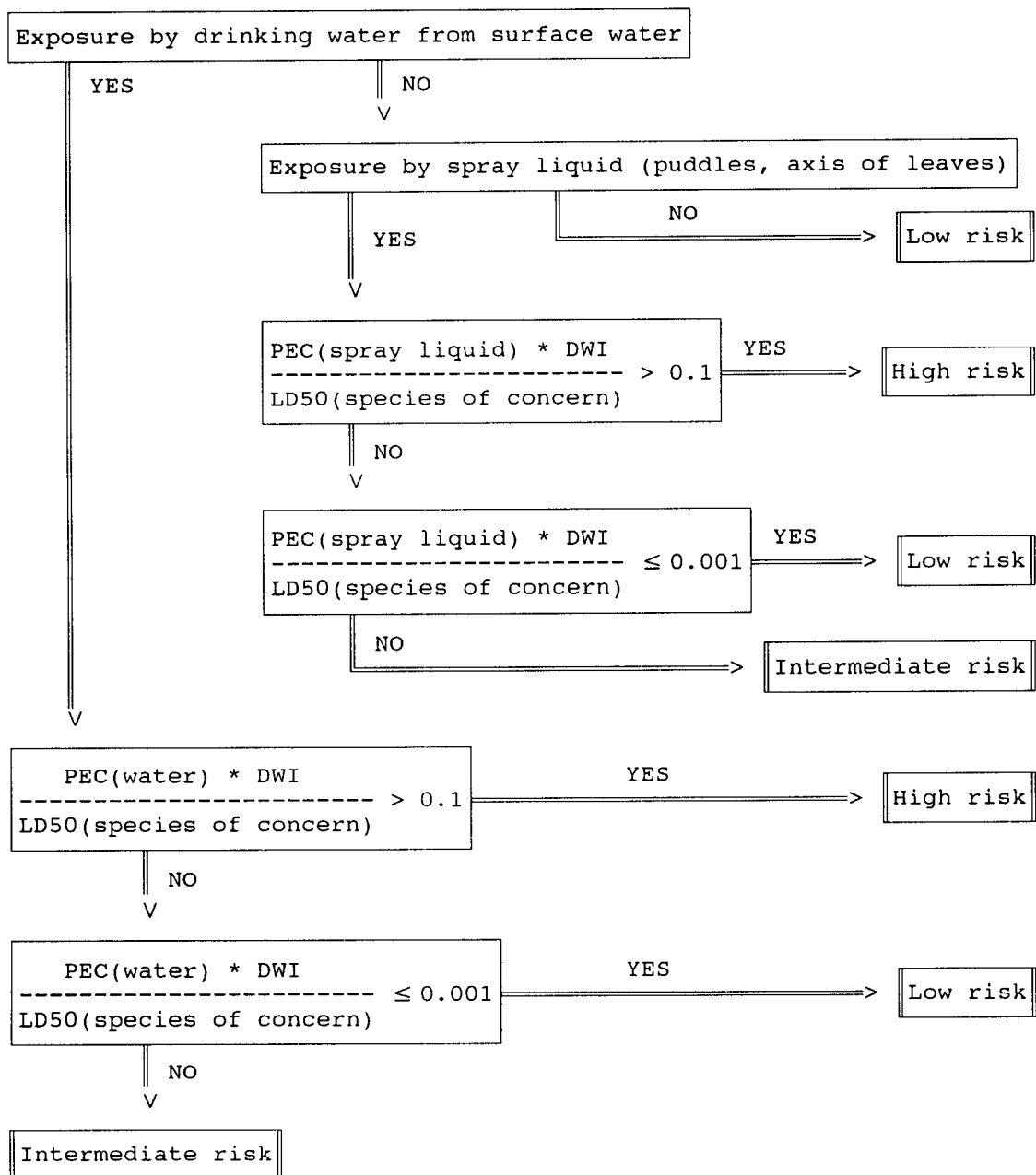
D' Exposure by drinking water from surface water



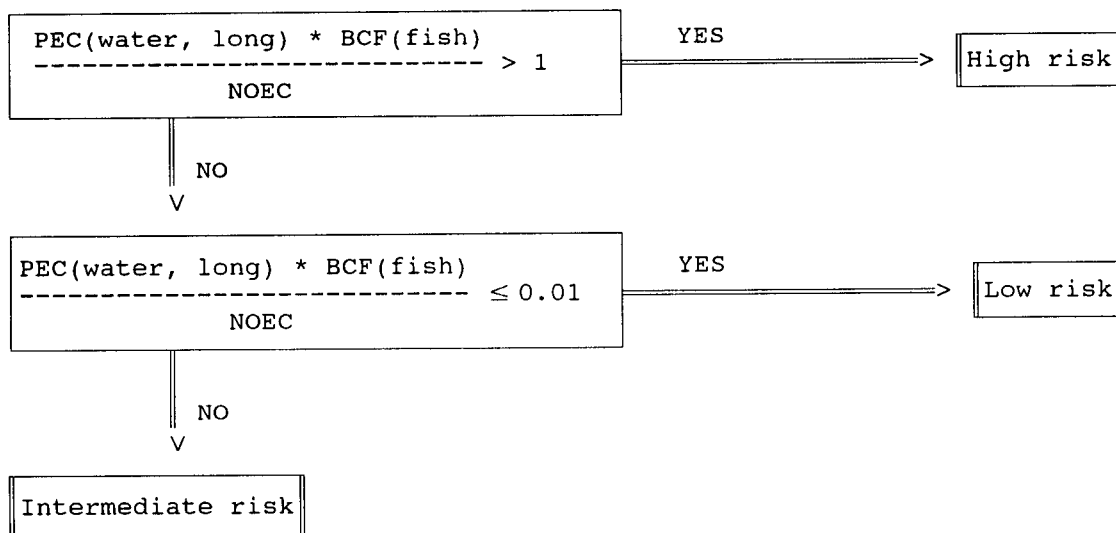
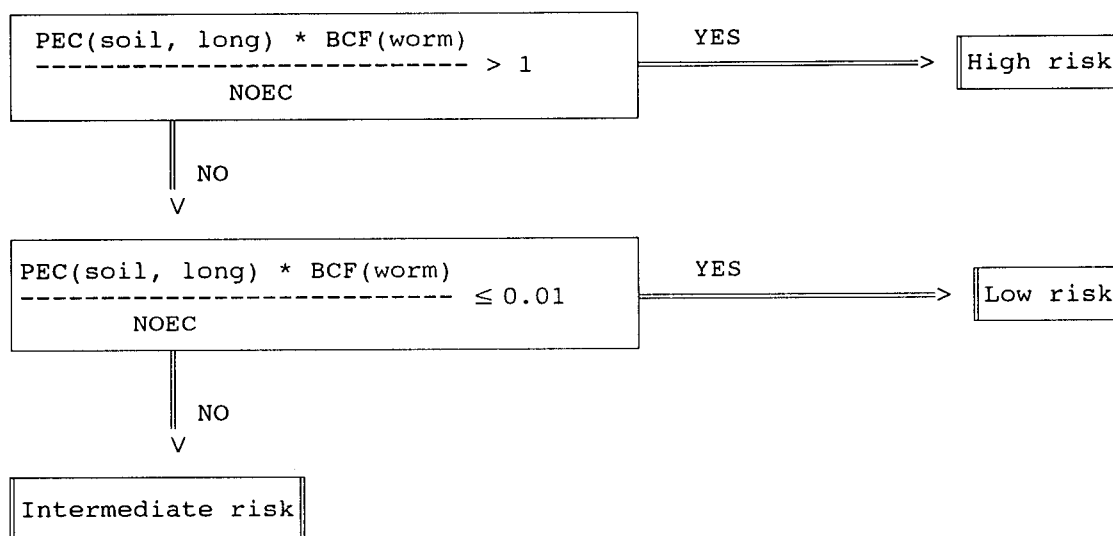
D" Exposure by spray liquid (puddles, axis of leaves)



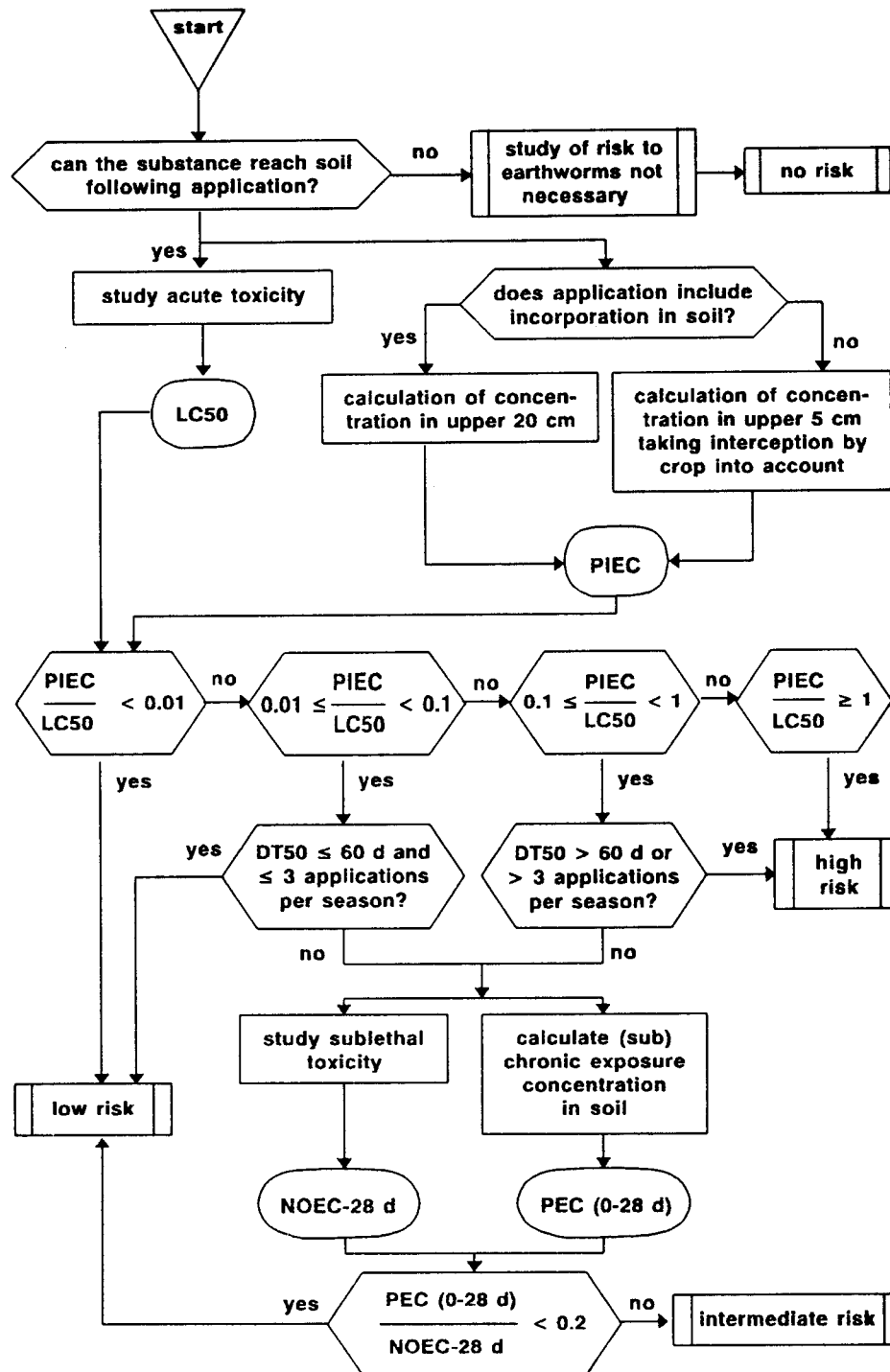
MODULE D Exposure by (drinking)water for mammals.



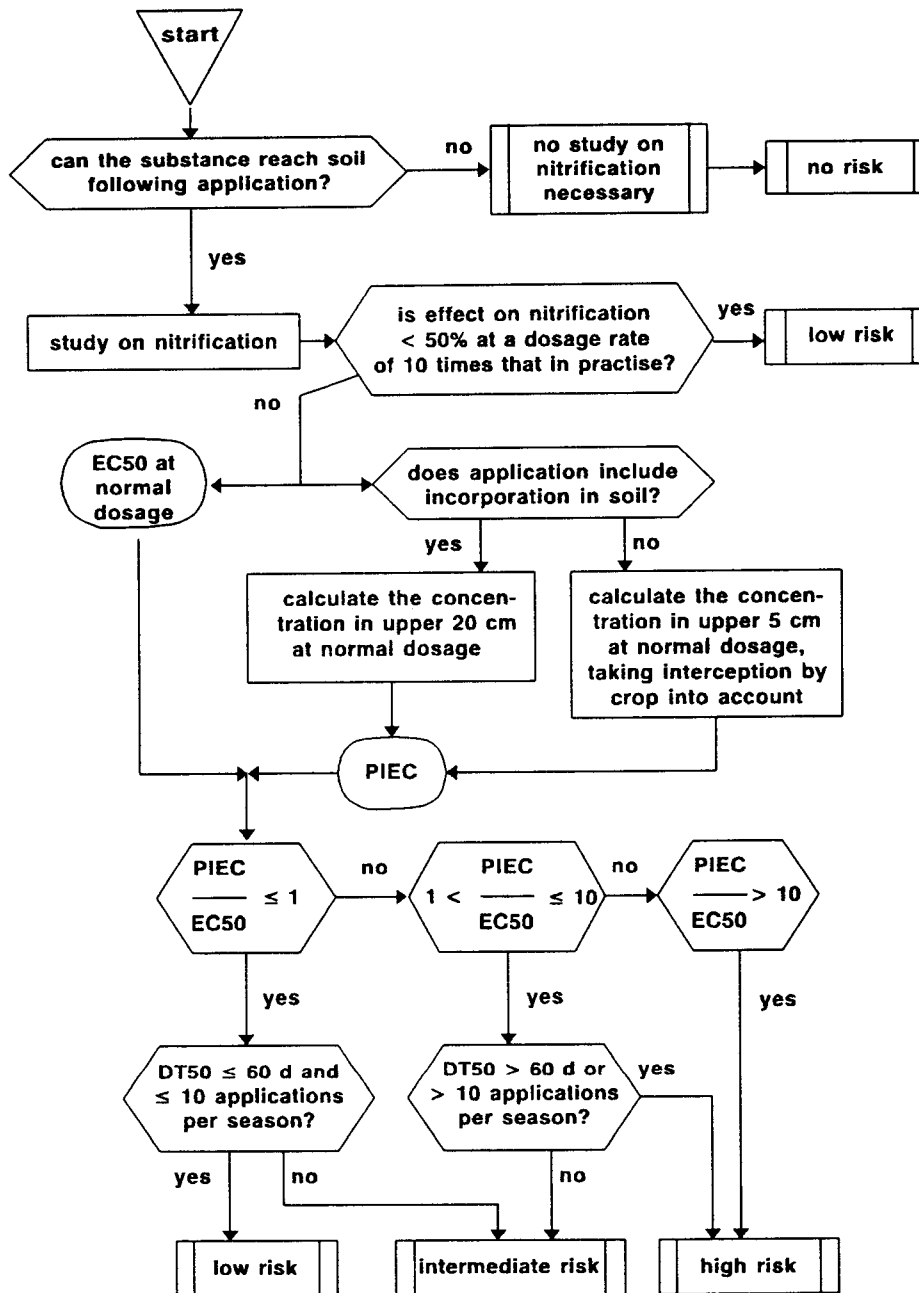
MODULE E Secondary poisoning for birds as well as mammals.

Fish as foodWorms as food

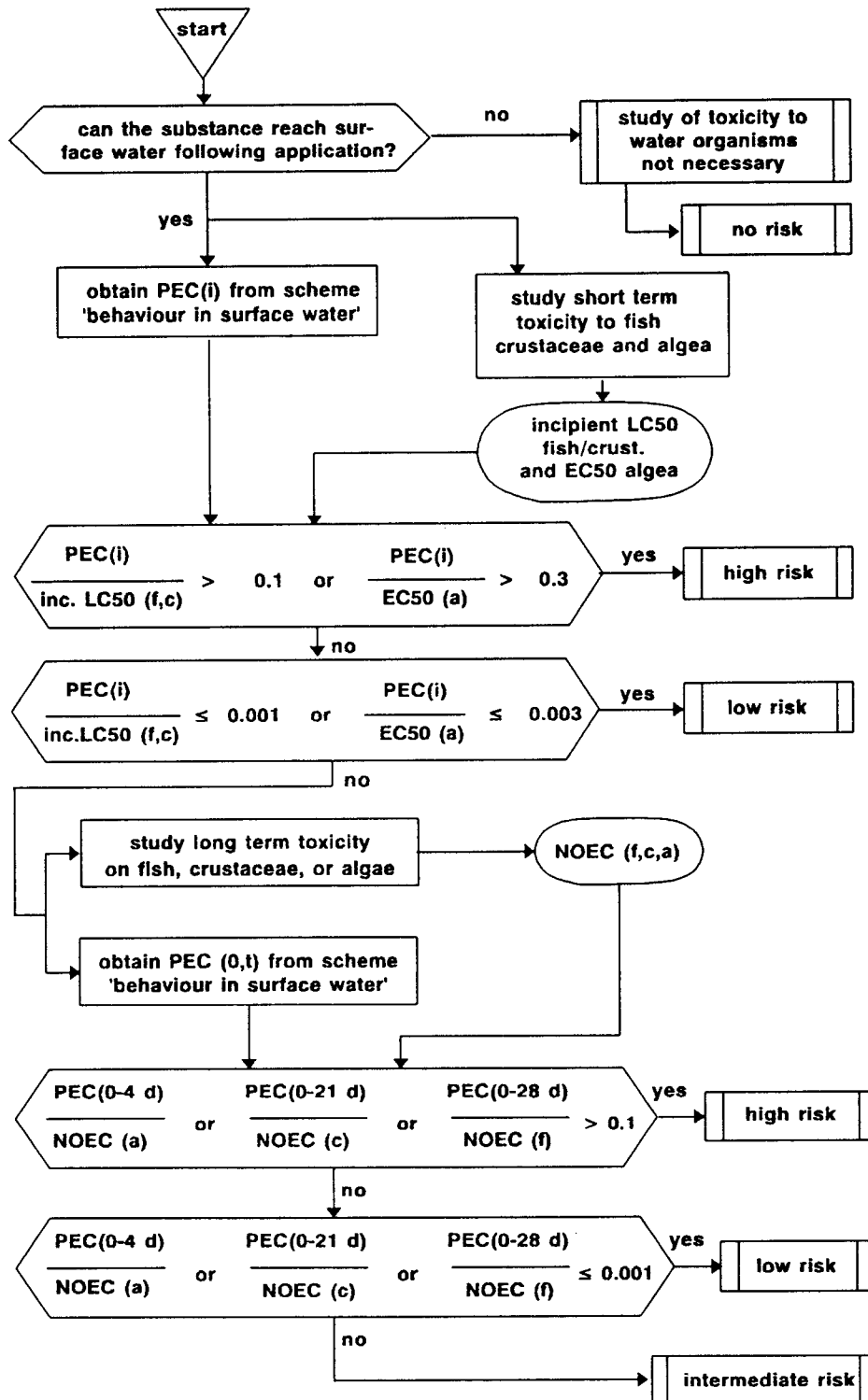
Appendix 9: Decision tree for earthworms

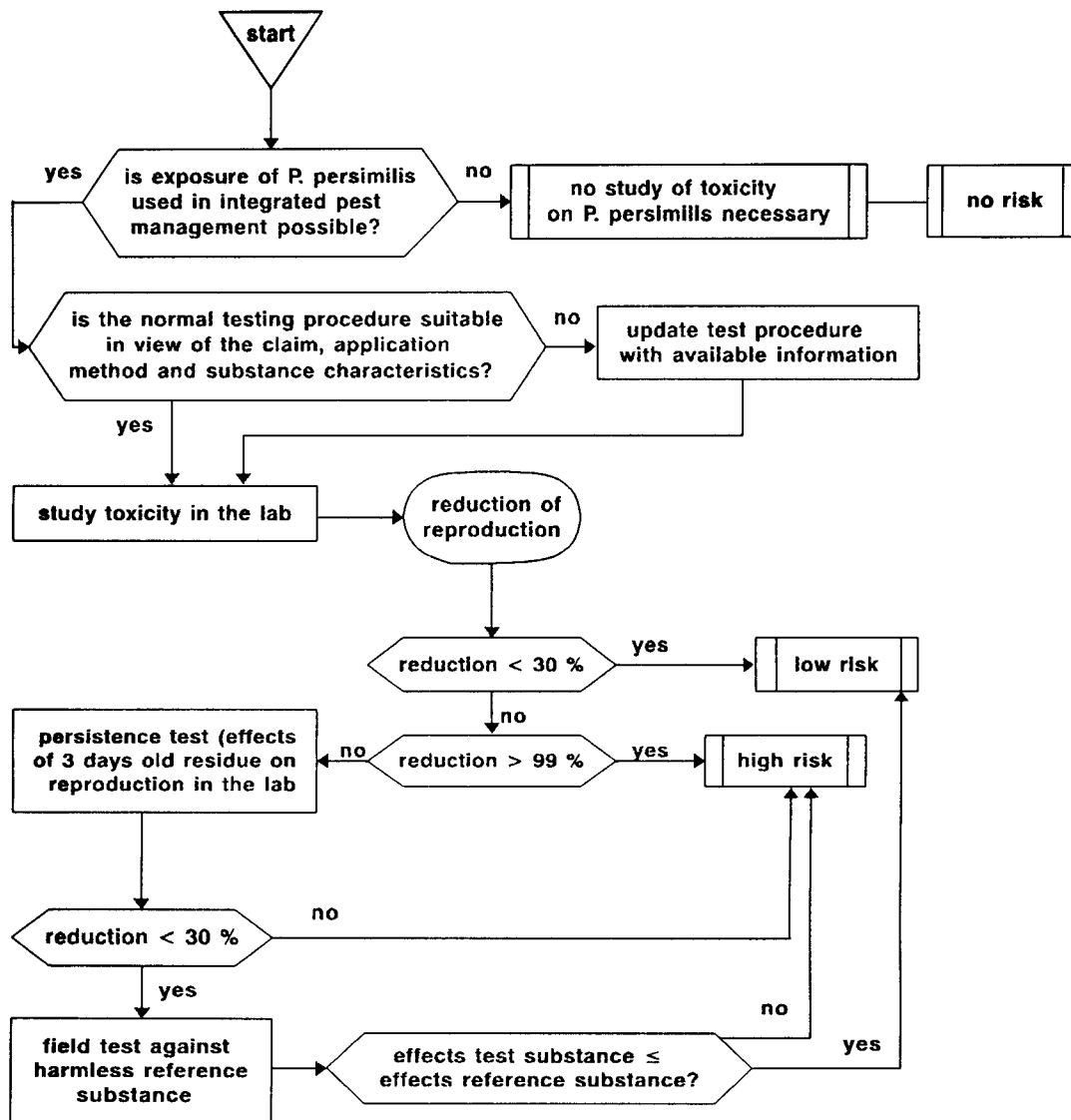


Appendix 10: Decision tree for nitrification

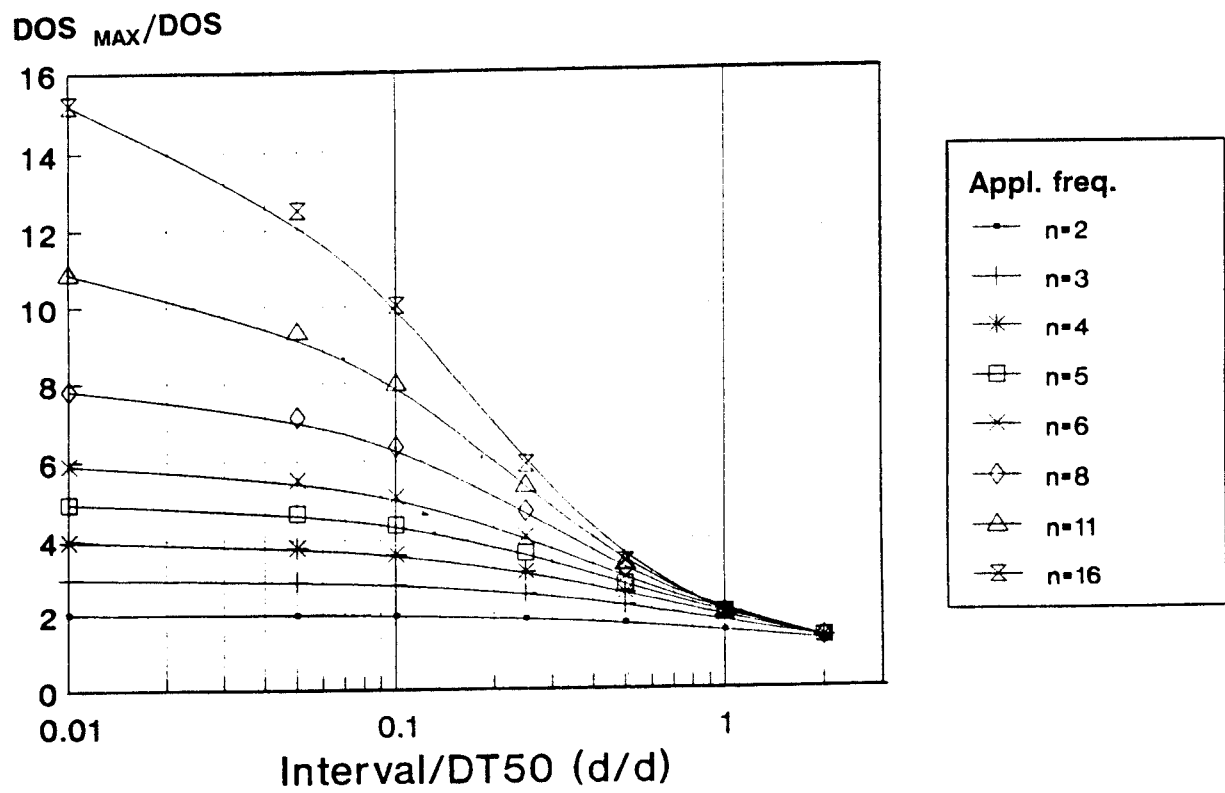


Appendix 11: Decision tree for water organisms

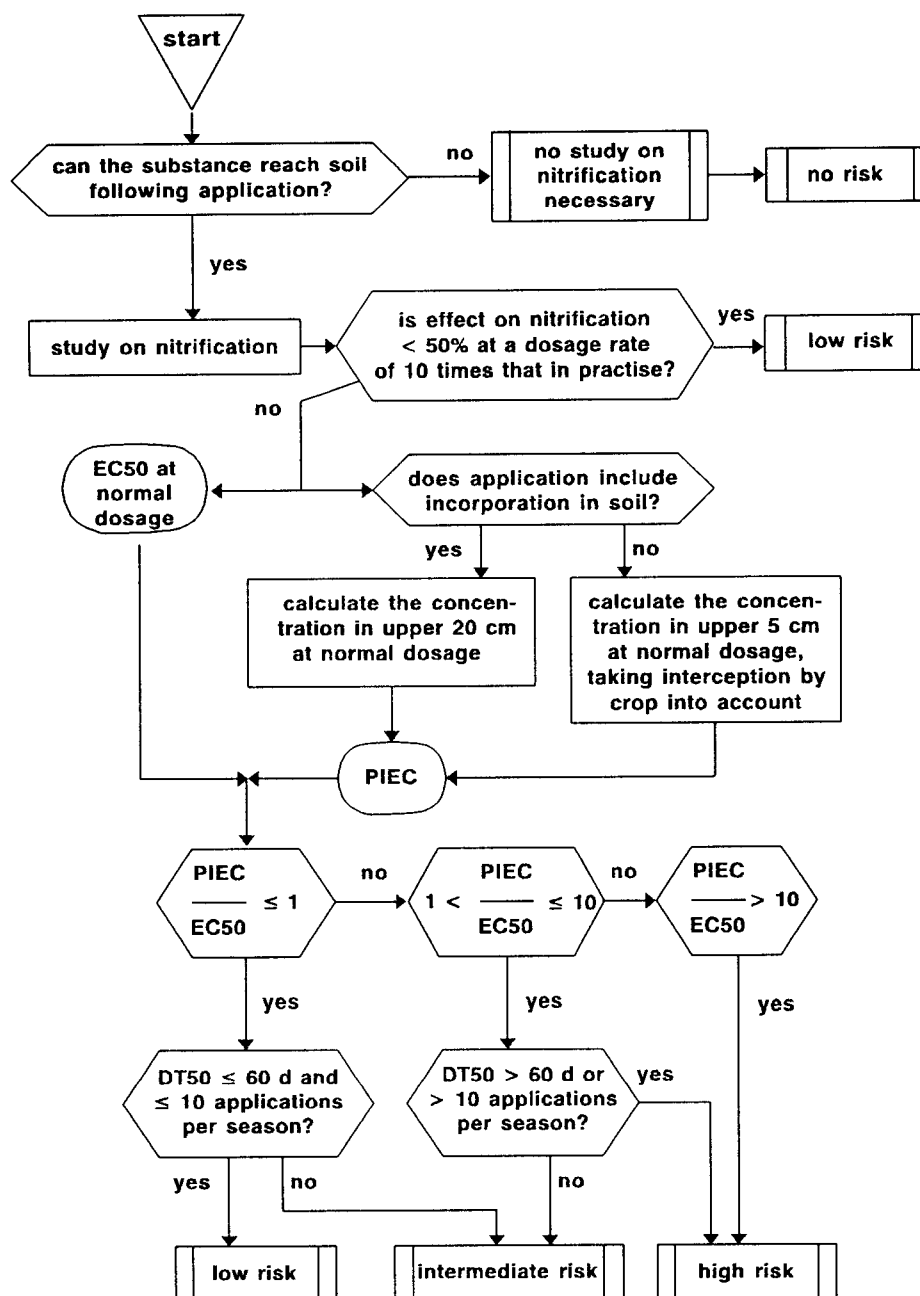


Appendix 7: Decision tree for *Phytoseiulus persimilis*

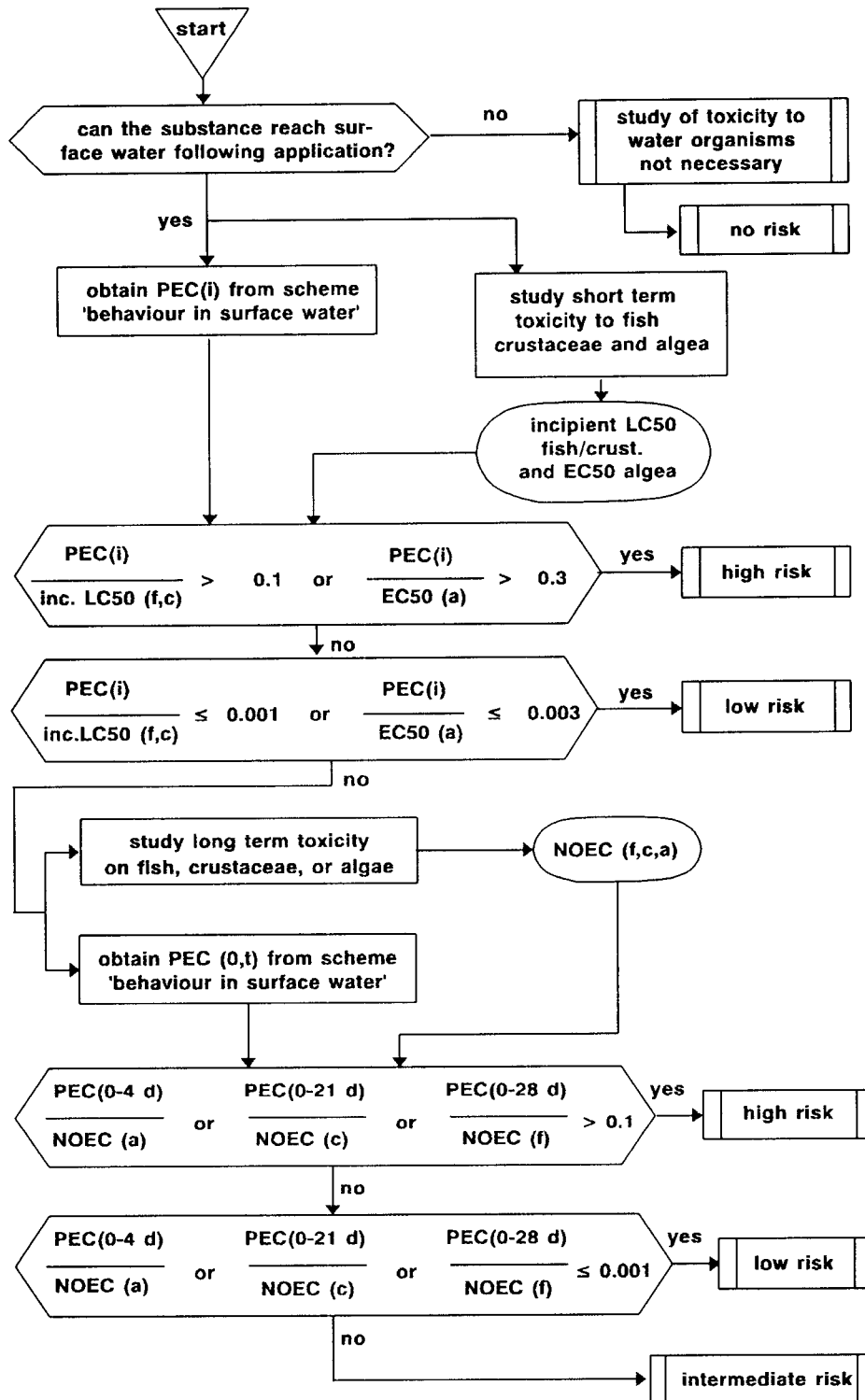
Appendix 1. Correlation between Dos_{max}/Dos and $Interval/DT50$ for several application frequencies



Appendix 10: Decision tree for nitrification



Appendix 11: Decision tree for water organisms



Appendix 9: Decision tree for earthworms

