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Modelling pesticide leaching at a regional scale in the Netherlands.

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PREFACE

This report describes the model GEOPESTRAS and the Information System on Pesticide Use (ISBEST). GEOPESTRAS is in fact a combination of the one-dimensional, process-oriented model PESTRAS (Freijer *et al.*, 1996) with a geographical information system. GEOPESTRAS has been developed to calculate the leaching of pesticides to the shallow groundwater on a regional scale in the Netherlands. It plays an important role in the development of Decision Support Systems for Pesticides. GEOPESTRAS is now used on a routine basis within the framework of the annual report 'State of the Environment'. The model has also been used for the evaluation of the Multi-Year Crop Protection Plan (MJP-G).

The development of the current version of PESTRAS was guided by a working-group of researchers from RIVM, SC-DLO, RIZA, TNO, and the University of Amsterdam. Aim of this working-group was to reach consensus about the underlying model. We wish to thank all participants of this working-group for stimulating discussions. The development of GEOPESTRAS was facilitated by C. van Heerden who helped with programming the interface between PESTRAS and the Information System. Thanks are further due to G. van Drecht and E. Scheper for deriving the grid-cell based maps of soil-type, organic matter content, and groundwater-depth-class. We wish to thank J.J.T.I. Boesten (SC-DLO, Wageningen) and B. Gottesbüren (BASF AG, Limburgerhof) for useful comments on a draft version of this paper.

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ABSTRACT

The leaching of pesticides to groundwater may introduce a risk to human health and ecosystems. For this reason, estimates are required of the magnitude of the leaching and the total area involved. A regional-scale pesticide leaching model, GEOPESTRAS, in combination with an Information System on Pesticide Use, ISBEST, was used to calculate the leaching of pesticides into the shallow groundwater for the Netherlands. Information on pesticide use was available at the community level. Calculations with GEOPESTRAS were performed for unique combinations of soil texture, organic matter content, groundwater-depth class, land use and climate. Model inputs were derived from these basic spatially distributed parameters using transfer functions. Spatial patterns of the pesticide leaching potential were obtained by combining the calculated results with geographic information. The number of unique combinations for which the model had to be run to get spatial patterns for the Netherlands could be reduced from 93,000 (which is the total number of relevant 500×500 m^2 grid cells in the Netherlands) to a manageable 897.

The calculated spatial pattern of pesticide leaching depended strongly on the pesticide properties. In the case of moderately degradable and moderately sorbing pesticides such as atrazine, the calculated concentration in the soil leachate was most dependent on the organic matter content. In the case of mobile pesticides (bentazone and hydroxy-chlorothalonile) a strong correlation was found with the mapped soil physical characteristics, whereas the concentrations of volatile pesticides depended strongly on groundwater level and soil physical properties. This demonstrates that general conclusions on the leaching potential cannot be drawn on the basis of results for a single pesticide, or a single parameter (e.g. organic matter content).

Peat soils were calculated to be invulnerable to pesticide leaching, whereas sandy and loamy soils with low organic matter content were very vulnerable (concentration often above 1 μg L^{-1}). The highest pesticide leaching was calculated for the 'Veenkoloniën' to the north-east, the flower-bulb area of the north-west and the sandy soils of the province of Noord-Brabant. The total calculated pesticide leaching amounted to 51,000 kg in the year 1993, of which 27,000 kg reached the deeper groundwater and 24,000 kg the surface water.

Key words: pesticides; leaching; soil; modelling; GIS; information systems; mapping; environment; vulnerability; groundwater; ISBEST; PESTRAS; GEOPESTRAS

SAMENVATTING

De aanwezigheid van bestrijdingsmiddelen in het grondwater introduceert een risico voor de volksgezondheid en ecosystemen. Om deze reden zijn schattingen nodig van de uitspoeling van bestrijdingsmiddelen naar het ondiepe grondwater. Hiervoor wordt een regionaal model van het gedrag van bestrijdingsmiddelen in de grond (GEOPESTRAS) in combinatie met het informatiesysteem bestrijdingsmiddelen (ISBEST) gebruikt. ISBEST levert gegevens over het gebruik van bestrijdingsmiddelen per gemeente. Berekeningen met GEOPESTRAS werden uitgevoerd voor unieke combinaties van bodemtype (textuur en organische-stofgehalte), grondwatertrap, landgebruik en klimaat. De invoer voor PESTRAS werd via vertaalfuncties afgeleid en een ruimtelijk beeld van de uitspoeling werd verkregen door de resultaten van de individuele berekeningen te combineren met geografische informatie. Het aantal combinaties waarvoor het model moest worden toegepast bedroeg 897.

Het berekende ruimtelijk beeld van uitspoeling was sterk afhankelijk van het type bestrijdingsmiddel. Bestrijdingsmiddelen die een gemiddeld gedrag wat betreft afbraak en sorptie vertonen (bijvoorbeeld atrazin), zijn sterk afhankelijk van het organische-stofgehalte. Mobiele stoffen (bentazon en hydroxy-chloorthalonil) vertonen een sterke correlatie met de textuurkaart, terwijl de uitspoeling van vluchtige stoffen (dichloorpropeen) sterk afhankelijk is van de diepte van het grondwater en bodemfysische eigenschappen.

In het algemeen werd berekend dat bestrijdingsmiddelen in veengronden niet of nauwelijks uitspoelden. De hoogste concentraties werden gevonden in zand- en leemgronden met een laag organisch-stofgehalte (concentratie vaak boven 1 $\mu g\ L^{-1}$). De grootste hoeveelheden bestrijdingsmiddelen spoelden uit in de Veenkoloniën, de Noord-Oost Polder, het bloembollengebied en de zandgronden van Noord-Brabant. De totale uitspoeling bedroeg in 1993 ongeveer 51000 kg, waarvan 27000 kg in het diepe grondwater en 24000 kg in het oppervlaktewater terechtkwam.

Trefwoorden: bestrijdingsmiddelen; bodem; modellering; GIS; Informatie-Systemen; kartering; milieu; gevoeligheid; grondwater; ISBEST; PESTRAS; GEOPESTRAS

1 INTRODUCTION

During the eighties it became clear that the total pesticide use per hectare arable land is high in the Netherlands compared to other western European countries (RIVM, 1989). In the same time, results of extensive groundwater monitoring programmes showed approximately 50 pesticides at observable concentrations in groundwater in western Europe and the USA (Leistra and Boesten, 1989; Hallberg, 1989; Kohsiek, 1991). For these reasons, the Dutch government released a declaration with the intent of reducing both the total pesticide use, and the emission of pesticides to groundwater, surface water, and the atmosphere. These objectives have been worked out in more detail in the Multi-Year Crop Protection Plan (LNV, 1991).

There are two ways of controlling pesticide leaching. The first is to reduce the total pesticide use. The above mentioned policy plan gives reduction targets (based on active ingredients used during the period 1984-1988) of 25-50 % in the year 1995, and 40-70 % in the year 2000. Given this objective, current policy is focused primarily on reducing the dependence on chemical pesticides, by stimulating organic and biodynamic agriculture, use of non-chemical pesticides, etc. The second way to control pesticide leaching is to ban the use of mobile pesticides. This policy is worked out by the Dutch Pesticide Registration Board.

The leaching of pesticides from the soil is affected by a number of processes, including degradation, sorption, plant uptake, transport and volatilization. The interaction between these processes is complex and non-linear (Boesten, 1991; Tiktak *et al.*, 1994b), making the use of simulation models in predicting pesticide leaching indispensable. In the Netherlands, the PESTLA model (Boesten and van der Linden, 1991) has been used for this purpose. The Pesticide Registration Board has defined a standard scenario for use with this model (i.e. one surface application of pesticide at a rate of 1 kg ha^{-1} in an initially pesticide free humic sandy soil, groundwater table at a depth of 1 m, application time on May 25, and weather data for a reference year). Pesticides are restricted or banned if the calculated maximum concentration of a pesticide between 1 and 2 m depth is above 0.1 μg L^{-1}, which is both the detection limit for many pesticides, and the EU drinking-water standard. Results from this standard analysis can be used to classify the leaching potential of pesticides relative to each other. However, it does not give information about the influence of soil type, groundwater depth, weather conditions, and management practises on pesticide leaching. A pesticide that poses a high leaching risk in a sandy soil may have a low leaching potential in a peat soil. A quantitative description of pesticide leaching on a regional scale requires the incorporation of these factors into the analysis.

From 1990 onwards attempts were made to assess spatial patterns of the vulnerability of soils to pesticide leaching on a regional scale (Bollen *et al.*, 1994; Kohsiek, 1991). These studies were based on extrapolating the standard scenario by adjusting the sorption constant according to differences in the organic matter content of the soils. However, the resulting spatial pattern does not account for differences in other factors, such as groundwater depth. Also in the US regional pesticide leaching models have been developed (Loague *et al.*, 1990; Petach *et al.*, 1991), which are often based on simplified models such as the GUS index (Gustafson, 1989) and CMLS (Nofziger and Hornsby, 1987). The disadvantage of these models is that they lack a physically based description of the underlying processes, so their use is limited to specific conditions. The use of the capacity model of water flow in CMLS, for example, is restricted to sandy soils with deep ground-water tables.

In 1995, a procedure has been proposed to map the vulnerability of soils to pesticide leaching in which all of the above mentioned factors ('basic spatially-distributed parameters') have been incorporated (Tiktak *et al.*, 1996). In this procedure, the physically based pesticide leaching model PESTRAS (Tiktak *et al.*, 1994; Freijer *et al.*, 1996) is directly applied to a number of unique combinations of these parameters. These unique combinations are assumed to be representative for one or more grid-cells or polygons within the area to be mapped (here referred to as 'mega-plots'). The number of mega-plots for which the model has to be run is dependent on the number of distinguished basic spatially-distributed parameters, on the spatial resolution, and on the number of classes for each basic parameter. Recently, PESTRAS was coupled to the Information System on Pesticide Use (ISBEST; Merkelbach *et al.*, in prep.) to obtain estimates of the actual pesticide loadings to the groundwater. This information will be used for mapping pesticide leaching within the framework of the annual reports 'State of the Environment' (RIVM, 1995a,b; RIVM, 1996a,b).

The general objective for this report is to present a procedure for the assessment of pesticide leaching on a regional scale, that can be applied within the framework of the annual State of the Environment. This procedure is based on the application of a pesticide leaching model on unique combinations ('mega-plots') of soil type, crop type, and weather conditions. The effect of these basic spatially-distributed parameters on pesticide leaching is described on the basis of results for four pesticides with contrasting properties, i.e. atrazine (2-chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine), bentazone (3-isopropyl-1*H*-2,1,3-benzothiadizin-4-(3*H*)-one 2,2-dioxide), a transformation product of chlorothalonile (4-hydroxy-2,5,6-trichloroisophtalonitrile), and cis-1,3-dichloropropene. Calculated regional patterns of pesticide leaching are shown for these four pesticides.

Finally, data are presented for the 18 pesticides that due to their use and properties are calculated to have a high ranking in leaching.

2 MODELS AND METHODS

2.1 Introduction

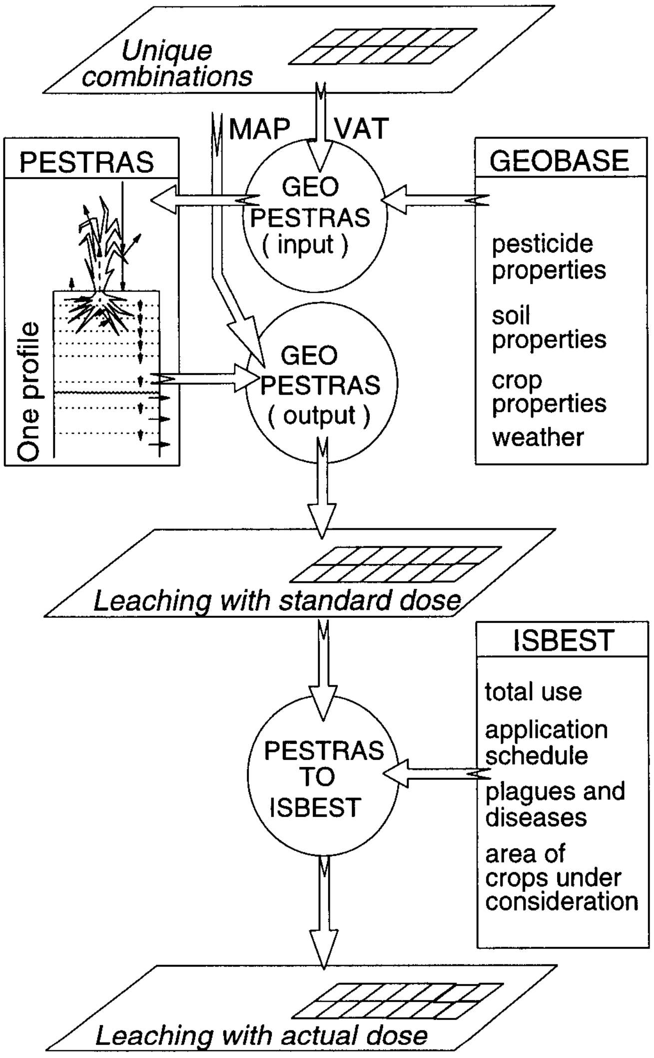


Figure 1 Overview of the PESTRAS-ISBEST information systems.

The assessment of the leaching of pesticides on a regional scale is carried out in two steps (Figure 1).

In a first step, the physically based pesticide leaching model PESTRAS (Tiktak *et al.*, 1994; Freijer *et al.*, 1996) is run to calculate the leaching of pesticides for unique combinations of soil type, groundwater depth class, crop-type and climate, using one standard dose of 1 kg active ingredient per hectare. Apart from soil fumigants such as 1,3-dichloropropene this is a quite realistic dose. Results include the maximum concentration of pesticide in shallow groundwater, and the fraction of pesticide leached.

In a second step, these two model outputs are combined with results from the Information System on Pesticide Use, ISBEST (Merkelbach *et al.*, in prep). ISBEST provides information on the total pesticide use per municipality, the area on which the pesticide has been applied, and the average dose on those parcels where the pesticide has actually been used. Multiplication of the fraction leached by the total pesticide use yields the total amount of pesticide leached. Multiplication of the maximum concentration by the average dose on treated parcels gives the actual concentration of pesticide. Combining this information with the area on which the pesticide has actually been used, the percentage of land where the maximum concentration of pesticide exceeds the EU drinking-water standard of 0.1 $\mu g\ L^{-1}$ can be calculated.

The remainder of this chapter describes the pesticide leaching model PESTRAS (section 2.2) and the Information System on Pesticide Use ISBEST (section 2.3). Section 2.4

describes the coupling of PESTRAS and ISBEST with a Geographical Information System.

2.2 The pesticide leaching and accumulation model PESTRAS v3.1

2.2.1 General overview

The vulnerability of geographic locations to pesticide leaching has been assessed with the process oriented model PESTRAS (PESticide TRansport ASsessment; Tiktak *et al.*, 1994a, Freijer *et al.*, 1996). Process oriented models have advantages, such as flexibility (the model can be used under a broad range of conditions), and the possibility of field-scale validation. PESTRAS is a one-dimensional, dynamic, multi-layer model for simulating transient flow, hydrodynamic dispersion, equilibrium sorption, transformation, volatilization and uptake of pesticides by plant roots in the unsaturated zone and the uppermost part of the saturated zone. PESTRAS is an extended version of the Pesticide Leaching and Accumulation (PESTLA) model (Boesten and Van der Linden, 1991), which is used for pesticide registration purposes. PESTRAS consists of three major submodels: (i) hydrology, (ii) heat transport, and (iii) pesticide transport, sorption, transformation and volatilization (Figure 2). Surface runoff is not considered, as this is a major process in a small part of the country only. Plant growth is considered to be a boundary condition to the model, and parameters relevant for water- and pesticide-uptake are input.

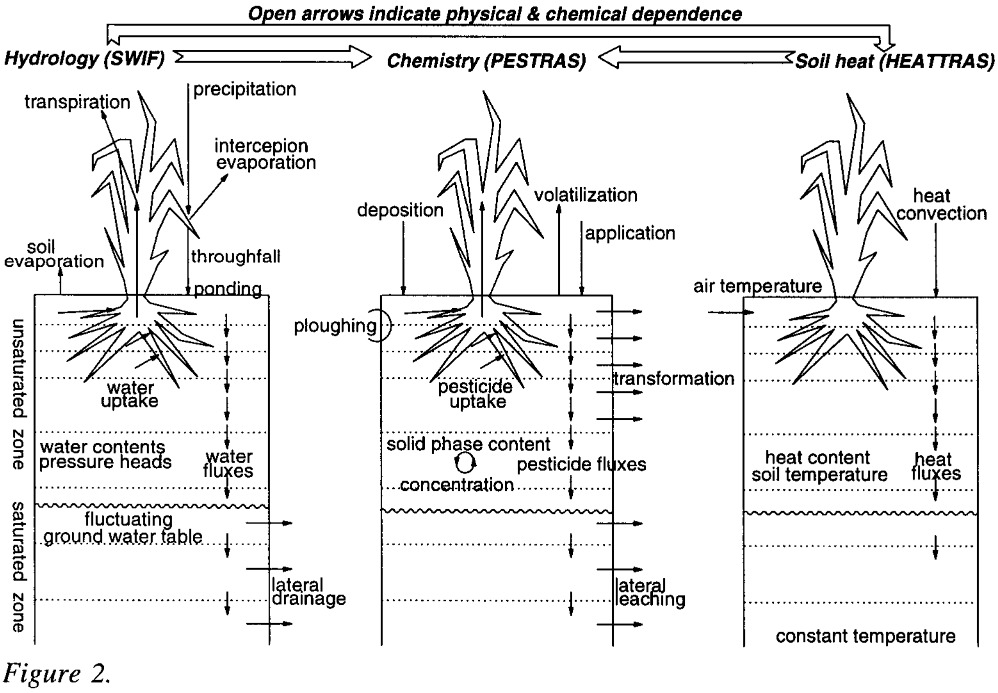


Figure 2.
Overview of the PESTRAS simulation model.

2.2.2 History of PESTRAS

Figure 3 gives an overview of pesticide modelling in the Netherlands. Currently, two models of pesticide leaching and accumulation are in use: PESTRAS 3.1 (Tiktak *et al.*, 1994; Freijer *et al.*, 1996) and PESTLA 2.3 (Boesten, 1993). In both models, process formulations for the fate of pesticides are based on version 1.1 of the model PESTLA (**Pest**icide **L**eaching and **A**ccumulation; Boesten and Van der Linden, 1991), which is still the official Dutch tool in pesticide legislation procedures. However, already in the seventies precursors of PESTLA existed. Soil hydrology is simulated in PESTRAS by the SWIF model (Tiktak and Bouten, 1992), which is an extended version of the ONZAT model (Van Drecht, 1983). The SWATRE model (Feddes *et al.*, 1978) is used in PESTLA. In PESTRAS, soil heat transport is simulated by the HEATRAS model, which is based on the heat exchange algorithm in the ILWAS model (Chen *et al.*, 1983). PESTLA either solves the heat diffusion equation or uses measured soil temperatures. The transport of pesticides in the gas phase is described by the GAS model (Freijer *et al.*, 1995). As PESTRAS and PESTLA have many common features, both models will be combined into one model in the near future (tentative name: Netherlands Leaching model for Pesticides).

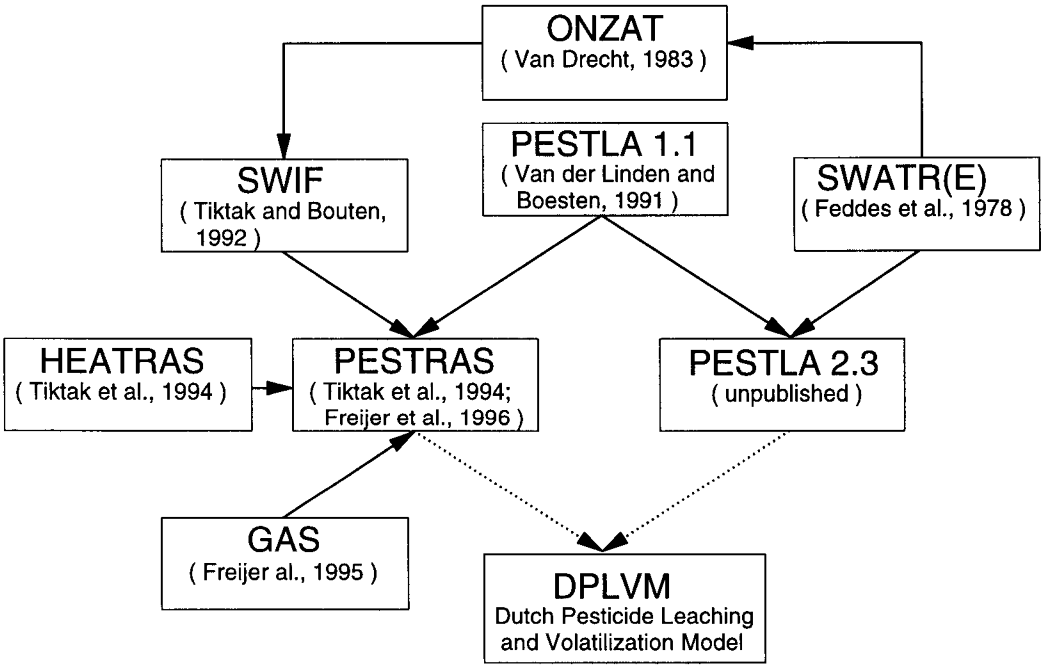


Figure 3
History of the PESTRAS model

2.2.3 Hydrology

The hydrological submodel (Tiktak and Bouten, 1992) uses a finite-difference method to solve the Richards equation:

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\,(\frac{\partial h}{\partial z}+1) \right) - S_w(h) \tag{1}$$

where C (m^{-1}) is differential water capacity, t (d) is time, z (m) is vertical position, h (m) is soil water pressure head, K (m d^{-1}) is unsaturated hydraulic conductivity, and S_w (d^{-1}) is a sink term accounting for root water uptake. In this study a time-dependent pressure head lower boundary condition has been used. The model is always run for one year prior to pesticide application to 'equilibrate' soil water fluxes with the calculated ground-water tabel.

The root water uptake, $S_{w,i}$ from a layer i is calculated from the potential uptake ($S^*_{w,i}$) and a dimensionless reduction function $f(h_i)$ for that layer (Belmans *et al.*, 1983):

$$S_{w,i} = f(h_i)\, S^*_{w,i} \tag{2}$$

The potential uptake from a layer is calculated by distributing the total potential transpiration T^* (m d^{-1}) over all soil layers according to the effective root length of a layer ($\Theta_i R_i$) expressed as a fraction of the total effective root length of the soil profile, $\Sigma(\Theta_i R_i)$:

$$S^*_{w,i} = T^*\,\frac{\Theta_i R_i}{\sum(\Theta_i R_i)} \tag{3}$$

where the saturation fraction Θ_i equals $\theta_i/\theta_{s,i}$, and θ_i and $\theta_{s,i}$ ($m^3\ m^{-3}$) denote actual and saturated water contents of layer i, respectively, R_i (m m^{-3}) is the root density of layer i, and

$$T^* = f_c\,(1 - e^{-0.6\cdot LAI})\, ET^* \tag{4}$$

with f_c (-) as an empirical crop factor, LAI ($m^2\ m^{-2}$) as the Leaf Area Index, and ET^* (m d^{-1}) as the potential evapotranspiration according to Makkink (1957). When the vertical distribution of potential transpiration is described with Eq. (3), preferential uptake from layers with high saturation fractions (Herkelrath *et al.*, 1977) is simulated.

The actual soil evaporation, E_s, is calculated according to the empirical relationship proposed by Black *et al.* (1969):

$$E_s = \beta\,.\left(\sqrt{t_d + 1} - \sqrt{t_d}\right) E^*_s \tag{5}$$

where E_s^* (m d^{-1}) is potential soil evaporation (ET^*-T^*), t_d (d) is time from the start of a drying cycle, and β (d$^{-1/2}$) is an empirical parameter. It is assumed that any drying cycle ends at a day with net precipitation $P_n > 1$ mm d^{-1}.

2.2.4 Heat transport

The model takes into account conductive and convective transport of heat in the soil:

$$\frac{\partial C_h T}{\partial t} = \frac{\partial}{\partial z}\left(\lambda \frac{\partial T}{\partial z} - J_w \rho_w H_w T\right) \tag{6}$$

where C_h (J m^{-3} K^{-1}) is the specific heat capacity, T (K) is temperature, λ (J m^{-1} d^{-1} K^{-1}) is the effective heat conductivity, J_w (m d^{-1}) is soil water flux, ρ_w (kg m^{-3}) is specific density of water, and H_w (J kg^{-1} K^{-1}) is the specific heat capacity of water.

2.2.5 Pesticide transport, transformation and sorption

The pesticide fate model considers a three phase one-dimensional soil in which a pesticide is present. The pesticide resides in all three phases of the system, i.e. an adsorbed phase, a dissolved phase and a gaseous phase. The total mass content of pesticide in the soil system, c^* (kg m^{-3}) is the sum of concentrations in these three phases:

$$c^* = \theta c + X \rho_b + \varepsilon Y \tag{7}$$

where θ (m^3 m^{-3}) is the volumetric soil water content, c (kg m^{-3}) is mass concentration in the liquid phase, X (kg kg^{-1}) is solid phase mass content, ρ_b (kg m^{-3}) is dry bulk density of the soil, ε (m^3 m^{-3}) is air-filled porosity, and Y (kg m^{-3}) is concentration in the gas phase. The total continuity equation for the three phases is:

$$\frac{\partial c^*}{\partial t} = -\frac{\partial J_l}{\partial z} - \frac{\partial J_g}{\partial z} + S_s + R_s \tag{8}$$

where J_l (kg m^{-2} d^{-1}) is the flux of pesticide in the liquid phase, J_g (kg m^{-2} d^{-1}) is the flux of pesticide in the gaseous phase, z (m) is vertical position, S_s (kg m^{-3} d^{-1}) is rate of plant uptake of the pesticide, and R_s (kg m^{-3} d^{-1}) is rate of transformation of the pesticide.

Vertical transport in the water phase

The flux of pesticide in the dissolved phase is described by:

$$J_l = qc - \theta(D_{dis} + D_{dif})\frac{\partial c}{\partial z} \tag{9}$$

where q (m d^{-1}) is the soil water flux, and D_{dis} (m^2 d^{-1}) and D_{dif} (m^2 d^{-1}) are the coefficients for dispersion and molecular diffusion, respectively. D_{dis} is calculated from:

$$D_{dis} = L_{dis}\left|\frac{q}{\theta}\right| \tag{10}$$

in which L_{dis} (m) is the dispersion length. The diffusion coefficient, D_{dif}, is calculated from:

$$D_{dif} = \lambda D_o \tag{11}$$

in which λ (-) is the tortuosity, and D_o is the diffusion coefficient in water.

Vertical transport in the gaseous phase

The flux of pesticide in the gas phase consists of a Fickian diffusion component and a pressure adjustment flux that accounts for convection and the presence of other gases such as N_2 and O_2 (Freijer and Leffelaar, 1995):

$$J_g = -D_{e,Fi}\frac{dY}{dz} + J_p \tag{12}$$

where $D_{e,Fi}$ (m^2 d^{-1}) is effective Fickian diffusion coefficient of gas in soil, and J_p (kg m^{-2} d^{-1}) is pressure adjustment flux, which is calculated from the mass balance of the gas phase assuming isobaric equilibrium (Freijer *et al.*, 1996).

The effective diffusion coefficient is reduced compared to the diffusion coefficient in free air:

$$D_{e,Fi} = Q D_{0,Fi} \tag{13}$$

where Q (-) is relative diffusion coefficient, and $D_{0,Fi}$ is effective Fickian diffusion coefficient of gas in free air. The relative diffusion coefficient is described according to Bakker and Hidding (1970):

$$Q = a(\varepsilon - \varepsilon_o) \tag{14}$$

where ε_o (m^3 m^{-3}) is the air-filled porosity at the pressure head corresponding to the air-entry value, and a (-) is an empirical constant. The diffusion coefficient of gas in air is calculated from the diffusion coefficient under reference conditions by:

$$D_{0,Fi} = D_{ref,Fi}\,(T/T_{ref})^{1.75}\,(p/p_{ref})^{-1} \tag{15}$$

where $D_{ref,Fi}$ (m^2 d^{-1}) is the effective Fickian diffusion coefficient of gas in free air under reference conditions, T (K) is temperature, and p (Pa) is air pressure.

Equilibrium distribution between the phases

Equilibrium sorption onto the soil solid phase is described with the Freundlich equation:

$$X = K_F \, c^{\,1/n} \tag{16}$$

where K_F ($\mathrm{m}^{3/n}$ $\mathrm{kg}^{-1/n}$) is the Freundlich sorption coefficient, and $1/n$ is the Freundlich exponent. The Freundlich coefficient is calculated from the coefficient for distributing the substance over organic matter and water, K_{om} (m^3 kg^{-1}) (Van der Linden and Boesten, 1991):

$$K_F = f_{om} K_{om} c_e^{\,1-(1/n)} \tag{17}$$

where f_{om} (kg kg^{-1}) is the mass fraction of organic matter, and c_e (kg m^{-3}) is the concentration at which K_F has been calculated (usually 1 g m^{-3}).

The dissolved and gaseous phases are assumed to be in equilibrium in accordance with Henry's law:

$$Y = K_H c \tag{18}$$

where K_H (m^3 m^{-3}) is Henry's partitioning coefficient.

Transformation of the pesticides

The transformation of a pesticide in the soil, R_s, is described with a first-order rate equation (Boesten and van der Linden, 1991):

$$R_s = f_T f_p f_z \frac{\ln(2)}{DT_{50}} c^* \tag{19}$$

where f_T, f_p and f_z (-) are reduction factors accounting for the influence of temperature, soil-water pressure head and depth in soil, DT_{50} (d) is the disappearance half-life under reference conditions (i.e. measured in freshly sampled top-soil at a temperature of 293 K, and at a soil water pressure head of -1 m), and c^* (kg m^{-3}) is the total content of pesticide in the soil system. The reduction factors are described by:

$$f_T = e^{(\gamma(T-T_{ref}))} \tag{20}$$

and

$$f_p = \min\left(1,(h_{ref}/h)^B\right) \tag{21}$$

where B (-) and γ (K^{-1}) are empirical parameters, T (K) is prevailing soil temperature, T_{ref} (K) is reference temperature (293 K), h (m) is soil-water pressure head, h_{ref} (m) is reference soil-water pressure head (usually -1 m), and min refers to 'minimum of'. The depth-in-soil function, f_z, accounting for depth distribution of microbial activity, is described through a table. PESTRAS includes algorithms for the simulation of parent-daughter relationships.

Uptake of pesticides

The uptake rate of a pesticide by plant roots from soil, S_s, is described by:

$$S_s = f_{uc} S_w c \tag{22}$$

where f_{uc} (-) is an empirical transpiration stream concentration factor, S_w (d^{-1}) is the sink term accounting for water uptake by plant roots, and c (kg m^{-3}) is mass concentration of pesticide in the liquid phase.

2.3 The Dutch Pesticide Information System ISBEST

ISBEST (Merkelbach *et al.*, in prep) has been developed to screen the use of pesticides in the Netherlands. Presently, the system contains data on the use of 337 officially registered formulations and 180 active ingredients in 14 so-called agricultural districts. The actual occurrence of plagues and diseases is described, based on representative surveys amongst 1500 farmers. Moreover, for 82 crops (table 1), and almost 600 combinations of crops and pests, the system describes how plant protection is carried out in practice. By combining this information with the spatial distribution of crop acreage, the use of pesticides is calculated on the scale of municipalities (Figure 4).

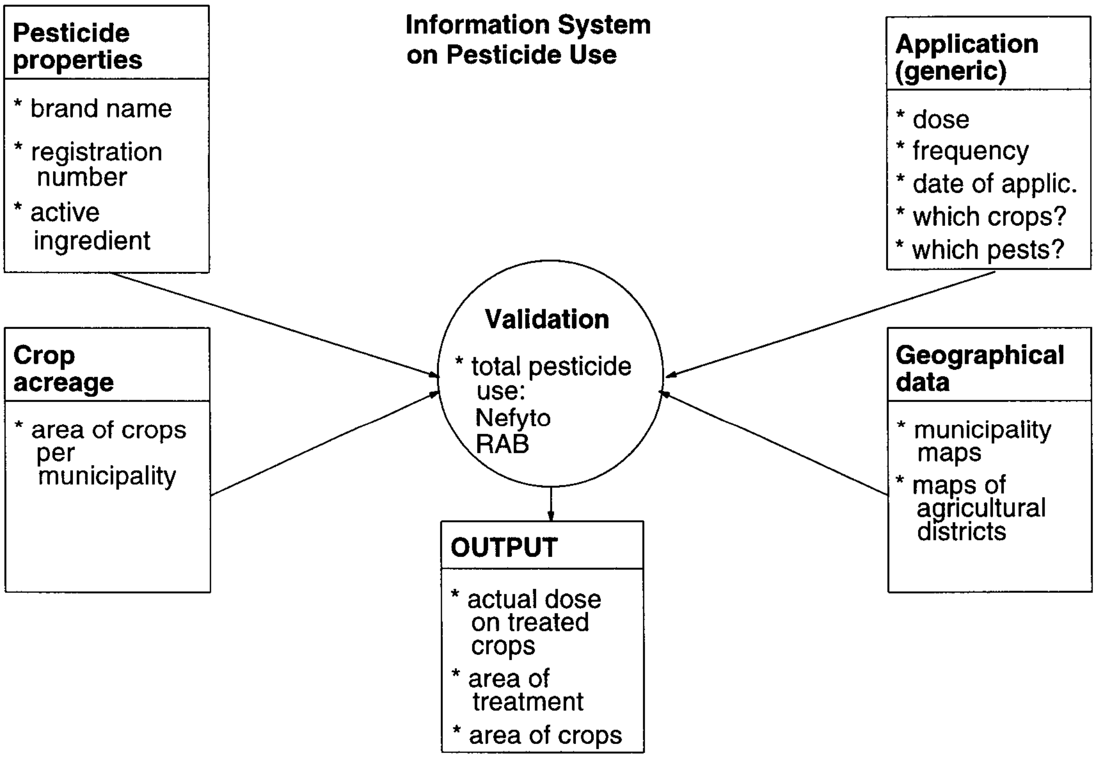


Figure 4
Overview of the Information System on Pesticide Use (ISBEST)

TABLE 1
Overview of crops distinguished in ISBEST

alfalfa	anthurium	apple-trees	asparagus
barley	beans	broad beans	Brussels sprouts
caraway seed	carrots	cauliflower	celeriac
chicory	chrysanthemum	cole	coleseed
conifers	corn	cucumber	daffodil
dianthus	endive	flax	freesia
gerbera	gherkin	gladiolus	grass
gypsophylia	hyacinth	iris	leek
lettuce	lilies	maize	mushrooms
oats	onion	orchid	oyster
paprika	pear-trees	peas	potatoes
public gardens	rose	rye	shrubs
spinach	strawberry	sugar beet	
tomatoes	tulips	wheat	

The practical information about plant protection plays a crucial role in the system. For each pest-crop combination, and for each pesticide, the following four parameters are available for each of the 14 districts:

- market position of individual pesticides (i.e. the share of each pesticide in controlling a certain plague or disease in a certain crop),
- actual dose and frequency of application,
- fraction of the total dose applied in spring,
- application type (spray, injection, granule application, fraction applied in immersion bathes, etc.).

These four parameters are available at the scale of the above mentioned agricultural districts. However, if a regional distinction cannot be made, one value is assumed for the country as a whole. The total use of each individual pesticide is calculated by summing the use of that particular pesticide over all combinations of pests and crops. An important step is the comparison of the so calculated total pesticide usage with sales figures. This validation has been carried out for 32 pesticides (table 2). Sales figures have been collected by the Plant Protection Service (PD) within the framework of the Regulation Administration Pesticides (so called RAB-figures), and by LEI-DLO and CBS. A maximum difference of 15% has been accepted, otherwise the original data are scaled to the RAB figures. The total pesticide use per agricultural district has been converted to an average dose per municipality on the basis of the digital version of the crop acreage database (CBS, 1993).

TABLE 2
Overview of 32 pesticides for which the total use has been compared with RAB sales figures.

aldicarb	atrazine	bentazone	captan
carbendazim	carbofuran	chloridazon	chlorothalonile
cis-dichloropropene	dicamba	dichlorovos	diuron
DNOC	fentinacetaat	glyphosate	lenacil
lindane	mancozeb	maneb	MCPA
mecoprop	metalaxyl	metam-sodium	metamitron
metolachlor	oxamyl	parathion-ethyl	pendimethalin
pirimicarb	propachlor	pyridate	zineb

2.4 Incorporation of PESTRAS into the GIS

2.4.1 Database development and database structure

The PESTRAS model contains 53 parameters, of which 30 depend either on soil type, crop type or climate. These parameters are stored in a GIS database. It is clear that organization of these parameters within the database is important to (Vaughan and Corwin, 1994): (i) establish a hierarchy, (ii) minimize the data requirement, and (iii) reduce the number of unique combinations (mega-plots) and computation time.

A first step in achieving these goals is to classify parameters as either 'spatially-distributed' or 'spatially-constant' (Figure 5). The reason for classifying a parameter spatially-constant is often obvious. Chemical properties, such as the disappearance half-life under reference conditions, and the coefficient for partitioning between water and organic matter are derived from standard experiments, and their values are assumed constant. Ambient air-temperature was considered spatially-constant as the variation across the Netherlands is small ($9 < t_{avg} < 10$ °C; t_{avg} is average annual temperature). This applies to both the climatic records, and the seasonal course of temperatures. Parameters such as the application schedule are assumed spatially-constant simply because it is the aim of our study to have the vulnerability assessment independent of management practices. Daily precipitation and evapotranspiration rates were obtained by combining maps of long-term (1961-1990) average annual precipitation and evapotranspiration with daily records from a reference site and year (relationship represented by dashed line). This calculation is only appropriate if the seasonal course of rainfall and evaporation shows comparable patterns across the area considered. This assumption holds for climatic records as shown by maps published by the Royal Netherlands Meteorological Institute (KNMI, 1972), but large deviations may occur for single years. In other words: more detailed weather data are required if one wants to calculate actual pesticide leaching rates for a particular year.

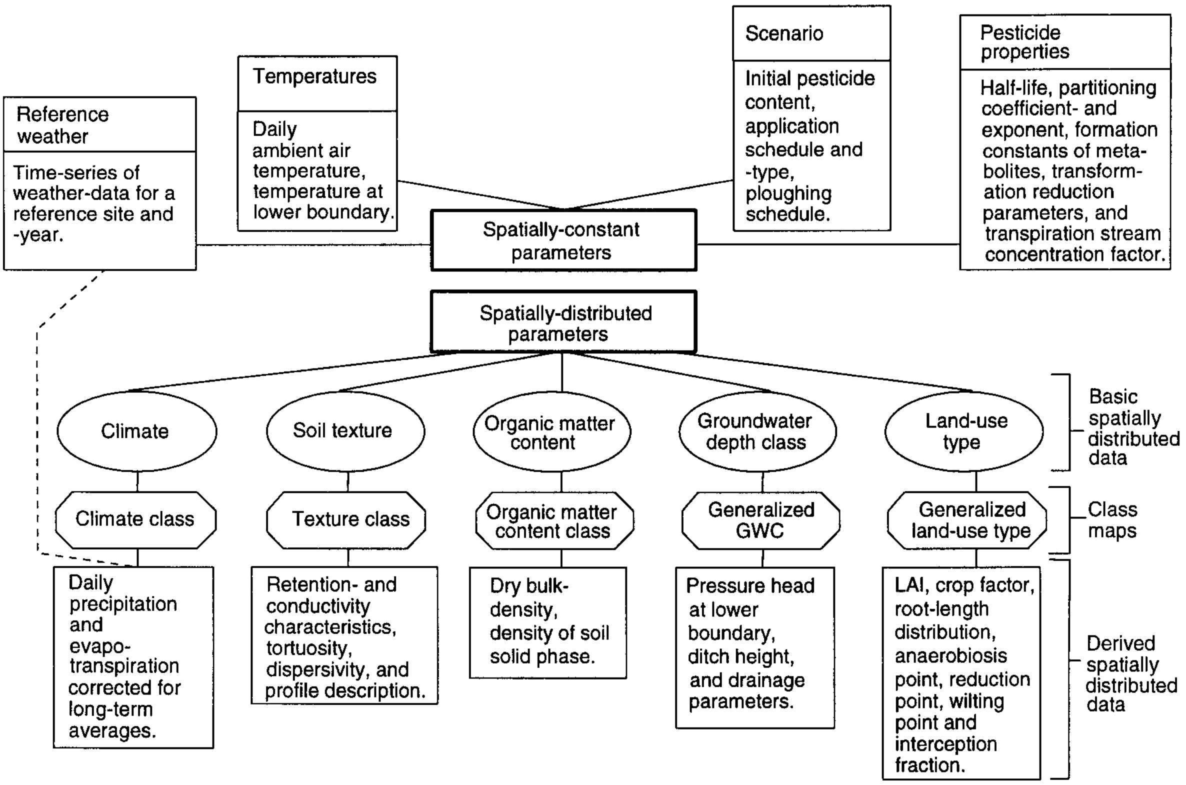


Figure 5.
Structure of the PESTRAS database. Lines indicate relationships.

A second reduction of the number of unique combinations for which PESTRAS had to be run was achieved by classifying the spatially-distributed parameters into basic spatially-distributed parameters and derived spatially-distributed parameters (Vaughan and Corwin, 1994). Derived spatially-distributed parameters were calculated, using a continuous (pedo)transfer approach (Bouma and van Lanen, 1987), a class (pedo)transfer approach (Wösten *et al.*, 1994; Wösten *et al.*, 1995), or they were obtained from literature. Details are given in the section on model inputs. The following spatially-distributed parameters were classified basic parameters: precipitation, potential evapotranspiration, land-use, groundwater-depth-class (GWC), organic matter content of the soil, and soil texture. These basic spatially-distributed parameters were processed to obtain grid maps with cell size 500×500 m^2. This grid cell size was chosen, because land-use inventories were carried out for this scale already in the early eighties, and it has become the Dutch standard for many nationwide inventories. Some of the basic grid maps were derived from other data-sources. For example, organic matter content, soil texture, and groundwater-depth-class were derived from the digital soil map of the Netherlands (De Vries, 1993; De Vries and Denneboom, 1993). However, as the derivation of these parameters from the soil map has involved some manual operations, it was decided not to include these relationships into the

PESTRAS database structure. In other words: The term 'basic parameter' only refers to the hierarchy *within* the PESTRAS database.

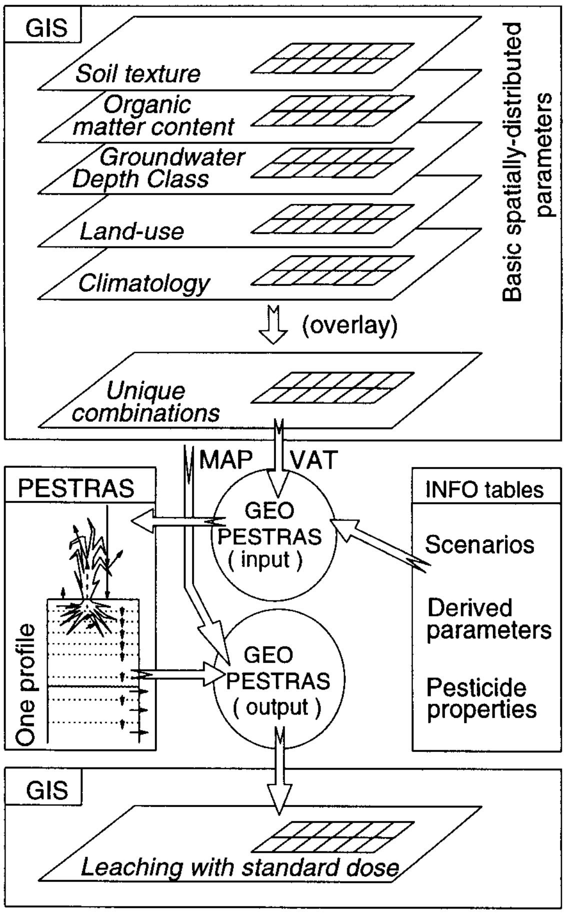


Figure 6
Incorporation of PESTRAS into the GIS

A final reduction of the number of unique combinations was achieved by classifying continuous basic data into a number of discrete classes. Ideally, the selection of classes is assessed by varying the number of classes and quantifying the sensitivity of vulnerability to such variations. In this study, however, the number of classes was based on preceding sensitivity analyses (Boesten, 1991; Tiktak *et al.*, 1994b), which showed high sensitivity of pesticide leaching to the organic matter content, and moderate sensitivity to precipitation, soil physical characteristics, crop-type, and ground-water depth. On the basis of these analyses, the number of classes was set highest for the organic matter content map. Once the number of classes was determined, these maps were sliced into classes of equal area, and the mean of each class was calculated.

2.4.2 Linkage between PESTRAS and the GIS

Figure 6 shows the linkage between the database and the model. ARC/INFO was the Geographical Information System utilized for the work discussed here. However, the methodology presented should be applicable to any GIS package that interfaces with a relational database. First, the basic maps were stored in the GIS, reclassified, and the mean value for each class was calculated (see preceding section). Then, the maps were combined to obtain a map of unique combinations or 'mega-plots'. The actual linkage between the model and the database was established through files (loosely coupled model; Burrough, 1996). An external program GEOPESTRAS reads, for each single model run, one record from the Value Attribute Table (VAT) containing information on soil-texture class, organic matter content class, land-use type, etc. Using this information, corresponding records in INFO tables were selected, and derived variables were calculated.

After combining all spatially-distributed parameters with spatially-constant parameters such as pesticide properties, the model was executed. Maps of calculated results were obtained by combining in the GIS the simulated values with the map of unique combinations.

2.4.3 Modelling the actual leaching of pesticides

In a second step, the two model outputs concentration in the 1-2 m soil layer and percentage leaching are combined with results from the Information System on Pesticide Use, ISBEST (Merkelbach *et al.*, in prep). ISBEST provides information on the total pesticide use per municipality, the area on which the pesticide has been applied, and the average dose on those parcels where the pesticide has actually been used. Multiplication of the fraction leached by the total pesticide use yields the total amount of pesticide leached. Multiplication of the maximum concentration by the average dose on treated parcels gives the actual concentration of pesticide. Combining this information with the area on which the pesticide has actually been used, the percentage of land where the maximum concentration of pesticide exceeds the EU drinking-water standard of 0.1 $\mu g\ L^{-1}$ can be calculated.

3 THE DATA-SET

3.1 Inputs to the model PESTRAS

3.1.1 Basic spatially-distributed parameters

Figure 7 shows the maps of basic spatially-distributed parameters, as included in the PESTRAS database.

Organic matter content classes

The organic matter content map included in the PESTRAS database was derived from an organic matter content map, based on the Soil Map of the Netherlands on a scale of 1:250,000. About 256 soil mapping units have been distinguished, distributed over the map in 6500 polygons (average size of the map polygons is 500 ha). The organic matter content map gives the minimum, average, and maximum organic matter contents for each mapping unit as a function of depth. It was obtained by combining geographical data from the Soil Map with profile description data stored in the Soil Information System (De Vries, 1993), using an area weighed averaging procedure. The average organic matter content of the upper meter was calculated, using a horizon thickness weighed averaging procedure. Finally, the organic matter content map was converted to a grid map (500×500 m^2), and sliced into 10 classes of equal area. The mean percentages of organic matter and the standard deviations for each distinguished class are: 0.4±0.03, 0.95±0.05, 1.22±0.06, 1.43±0.06, 1.58±0.07, 1.8±0.2, 2.06±0.3, 3.01±1, 6.62±6, and 33.0±17.

Soil texture classes

The map of soil physical characteristics included in the PESTRAS database was derived from the basic map of physical characteristics according to the 'Winand Staring Soil Series' (Wösten *et al.*, 1994). In its turn, this map was derived from the soil texture and organic matter content maps of the topsoil (upper 10 cm), and from the soil codes at the 1:250,000 digital soil map, using a program written in Arc Macro Language (AML). The soil texture map included information on clay content, silt content and sand content, and on the median particle size of the sand fraction (M_{50}). The soil texture map was derived in much the same way as the basic organic matter content map. The final map was created by aggregation. Classes were aggregated to one class if they showed comparable soil physical characteristics, or when the relative area of the individual classes was small. This yielded a total number of nine classes (table 3).

TABLE 3

Relative area, clay fraction, silt fraction, median particle size, and organic matter content for the nine units at the map of soil physical characteristics included in the PESTRAS database.

Name	Code[a]	Area (%)	f_{clay}[b] (%)	f_{silt}[b] (%)	M_{50}[b] (μm)	f_{om}[b] (%)
Coarse sand	B5	4	0-8	-	210-2000	0-15
Loam-poor fine sand	B1	21	0-8	0-10	0-210	0-15
Loamy fine sand	B2-B4	26	0-8	10-50	0-210	0-15
Light sandy clay	B7-B8	13	8-18	-	-	0-15
Heavy sandy clay	B9	11	18-25	-	-	0-15
Clay	B10-B12	8	25-100	-	-	0-15
Loam	B13-B14	2	-	50-100	-	0-15
Peat	B15-B18	10	-	-	-	15-100
glacial till	B6	5	-	0-50	50-2000	0-15

[a] Refers to the topsoil in the 'Winand Staring Soil Series' (Wösten, 1994).

[b] f_{clay} is clay fraction, f_{silt} is silt fraction, f_{om} is organic matter content, and M_{50} is median particle size of the sand fraction.

Ground-water-depth classes

Long-term average minimum and maximum groundwater depths are represented at the Soil Map of the Netherlands as so called groundwater-depth-classes (GWC). Predominant groundwater-depth-classes for each 500×500 m^2 grid cell were derived from the 1:50,000 digitized soil map (De Vries and Denneboom, 1993). The original groundwater-depth-classes were reclassified into six classes (table 4), which correspond to the major classes at the 1:250,000 Soil Map.

TABLE 4

Groundwater depth classes for the six units at the groundwater depth map included in the PESTRAS database.

Groundwater table[a]	GWC[b]	Area (%)	*MHW* (m)	*MLW* (m)
Very shallow	I, II	13	0.1	0.5
Fairly shallow	III	11	0.2	1.1
Moderately deep	II*, III*, V, V*	26	0.3	1.4
Fairly deep	IV, VI	34	0.6	1.6
Deep	VII	9	1.0	2.0
Very deep	VII*	7	2.0	3.0

[a] General classification at the 1:250,000 Soil Map of the Netherlands

[b] Groundwater-depth class at the 1:50,000 Soil Map of the Netherlands

[c] *MHW* is mean highest water table, and *MLW* is mean lowest water table

Land-use

Information on land-use types based on LANDSAT images were available for 25×25 m^2 grid cells (Thunnissen *et al.*, 1992). Using the information of 400 25×25 m^2 grid-cells, the relative area of various agricultural crops was calculated for each of the 500×500 m^2 grid cells used in this study. All arable crops were taken together, and finally two classes were distinguished: meadows (61% of total agricultural area) and arable land (39% of total agricultural area). The final land-use map is assigned the dominant of these two land-use types.

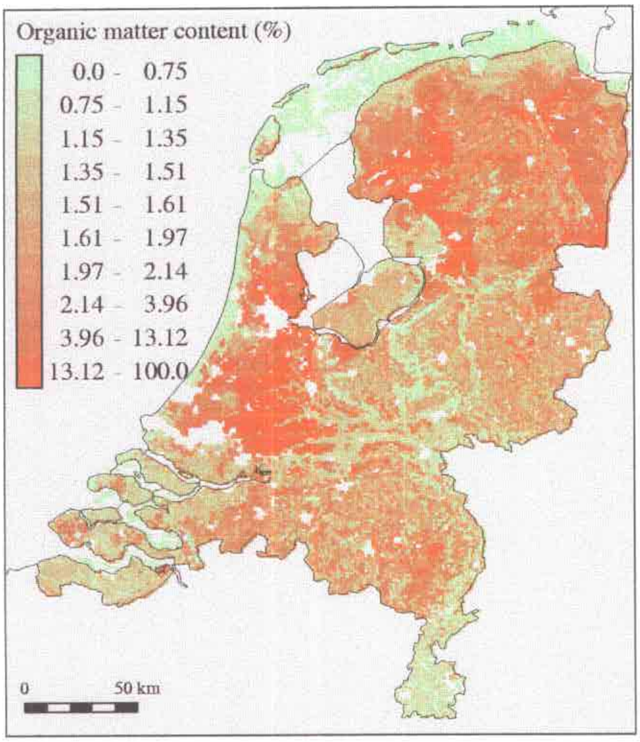
Precipitation

The geographic distribution of the long-term averages of precipitation for the period 1961-1990 was based on measurements at 172 precipitation observation stations. Because the precipitation stations were not uniformly distributed across the Netherlands, averages of precipitation were interpolated from the precipitation stations onto a uniform grid (500×500 m^2), using an inverse-distance-squared spatial interpolation algorithm. The continuous map thus obtained was sliced into a map with four classes of equal area: $P < 764$ mm a^{-1} (mean of class is 748 mm a^{-1}, and standard deviation is 18 mm a^{-1}), $764 \le P < 794$ mm a^{-1} (779±13), $794 \le P < 819$ mm a^{-1} (806±10) and $P \ge 819$ mm a^{-1} (843±24). The spatial pattern of precipitation amount is strongly affected by the North Sea to the West, and by differences in elevation.

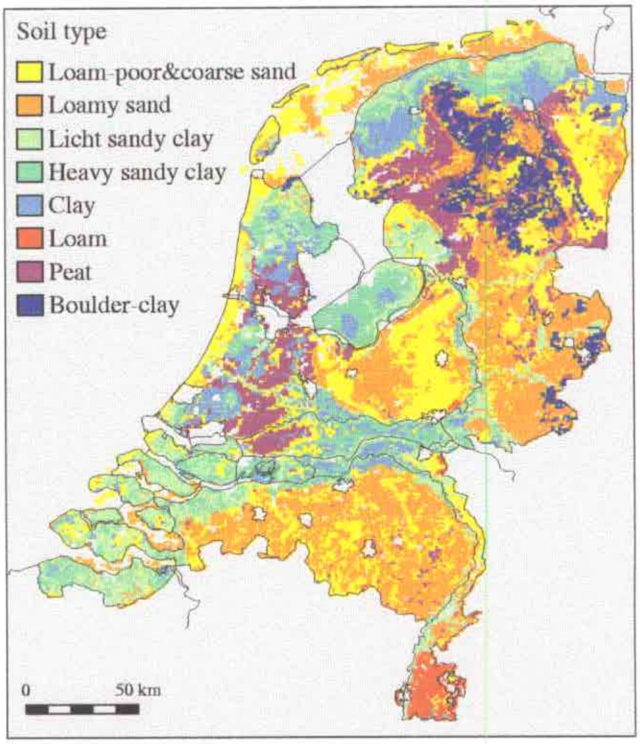
Evapotranspiration

The spatial pattern of the long-term averages of the potential evapotranspiration (1961-1990) was derived from evaporation figures published by the Royal Netherlands Meteorological Institute. These figures were based on observations at the 15 major weather stations. A drawback of this observational network is that the coastal area is poorly represented. For this reason, additional points were added in the Western and Northern parts of the Netherlands, based on observations of sunshine duration published in the climatic atlas of the Netherlands (KNMI, 1972). The point data were interpolated onto a uniform grid (500×500 m^2), using the above mentioned interpolation routine, and sliced into two classes with equal area, i.e. $ET^* < 547$ mm a^{-1} (mean value within class is 533 mm a^{-1}, and standard deviation is 13 mm a^{-1}) and $ET^* > 547$ mm a^{-1} (565±17).

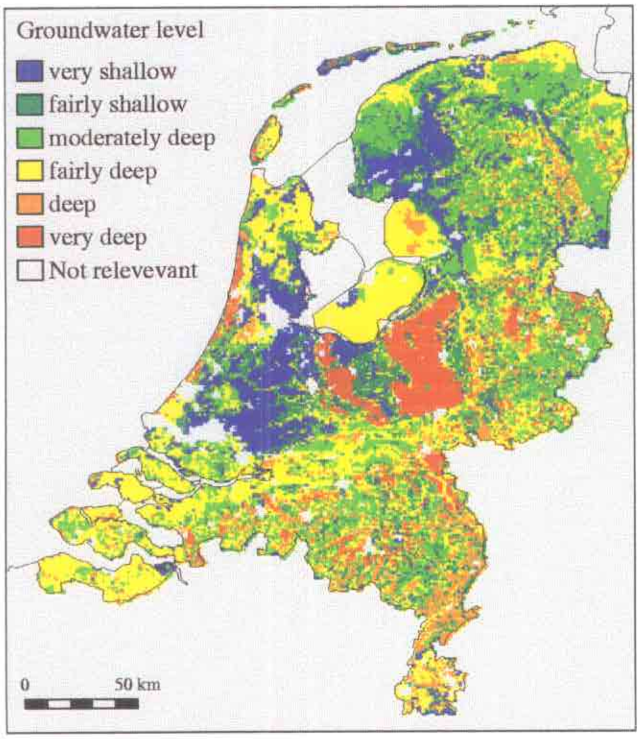
Organic matter content (%) of the upper meter of the soil profile. Source: Soil Map 1:250,000.



Soil texture classes according to the Winand Staring Soil Series. Source: Soil map 1:250,000.



Groundwater-depth-class. Based on the 1966 classification. Source: 1:50,000 Soil Map.



Long-term average precipitation (1961-1990). Source: KNMI.

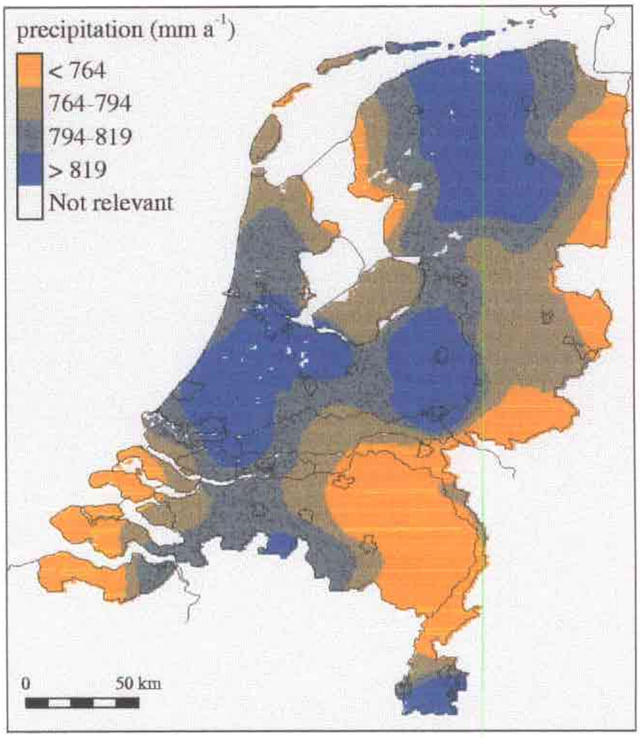


Figure 7

Maps of independent spatially-distributed parameters.

3.1.2 Derived spatially-distributed parameters

Daily weather conditions

Daily precipitation and evapotranspiration rates were obtained by combining the maps of long-term (1961-1990) average annual precipitation and evapotranspiration with daily records from a reference site and year:

$$P_d = P_{d,ref} \frac{P_a}{P_{a,ref}} \quad \text{and} \quad ET^*_d = ET^*_{d,ref} \frac{ET^*_a}{ET^*_{a,ref}} \tag{23}$$

where the suffix *ref* refers to a reference meteorological record, and *d* and *a* refer to daily and annual, respectively. Reference meteorological conditions were those observed in 1980 in De Bilt, situated in the centre of the Netherlands. Notice that Eq. (23) can only be applied for areas within one climatic zone, where the seasonal distribution of rainfall and evaporation shows comparable patterns across the area.

Crop properties

The most important crop dependent parameters are the Leaf Area Index (*LAI*), the rooting depth (R_{max}), and the crop factor (f_c). All these parameters are time-dependent (Table 5).

TABLE 5
The Leaf Area Index (*LAI*), crop factor (f_c), and rooting depth (R_{max}) on four selected times within the growing season.

Crop type	*LAI* (m^2 m^{-2})				f_c (-)				R_{max} (m)			
	Day of year				Day of year				Day of year			
	120	180	210	270	120	180	210	270	120	180	210	270
grass	1.5	2.5	3.5	3.5	1.0	1.0	1.0	0.9	0.2	0.2	0.2	0.2
arable land[a]	0.0	1.0	3.5	3.5	0.0	1.3	1.2	1.2	0.0	0.2	0.4	0.4

[a] Properties for maize

Depth distribution of organic matter content

The depth distribution of the organic matter content was calculated for each organic matter class according to:

$$f_{om,i} = f_{om,ref,i} \frac{f_{om,avg}}{f_{om,ref,avg}} \tag{24}$$

where $f_{om,i}$ (-) refers to the organic matter content of soil layer *i*, $f_{om,avg}$ (-) refers to the average organic matter content of the upper meter, and the suffix *ref* refers to a reference profile. The reference profile is a humic sandy soil profile with 4.7% of organic matter in the top 0.3 m, 0.8% in the 0.3-0.5 m soil layer, 0.1% in the 0.5-1.0 m soil layer, and zero below 1 m.

Soil physical characteristics

Soil hydraulic properties are represented in PESTRAS as (van Genuchten, 1980):

$$\theta(h) = \theta_r + \frac{(\theta_s - \theta_r)}{[1+(\alpha|h|)^n]^m} \tag{25}$$

and:

$$K(h) = K_s \frac{\{1-(\alpha|h|)^{n-1}[1+(\alpha|h|)^n]^{-m}\}^2}{[1+(\alpha|h|)^n]^{m/2}} \tag{26}$$

where θ_s (m^3 m^{-3}) is saturated volumetric water content, θ_r (m^3 m^{-3}) residual water content, α (m^{-1}) reciprocal of the air entry value, K_s (m d^{-1}) saturated hydraulic conductivity, n (-) a parameter, and m = 1-1/n.

TABLE 6

Parameters of the Mualem-Van Genuchten functions to describe the soil physical properties.

Soil type	Soil Layer	Code[a]	θ_r (m^3 m^{-3})	θ_s (m^3 m^{-3})	α (m^{-1})	n (-)	K_s[b] (m d^{-1})
Loam-poor	< 0.5 m	B1	0.43	0.01	2.49	1.507	0.478
fine sand	> 0.5 m	O1	0.36	0.01	2.24	2.167	1.699
Loamy	< 0.5 m	B2	0.02	0.43	2.27	1.548	0.593
fine sand	> 0.5 m	O2	0.02	0.38	2.14	2.075	0.942
Light sandy	< 0.5 m	B8	0.00	0.43	0.96	1.284	1.729
clay	> 0.5 m	O9	0.00	0.46	0.94	1.400	0.586
Heavy	< 0.5 m	B9	0.00	0.43	0.65	1.325	1.729
sandy clay	> 0.5 m	O10	0.00	0.49	1.07	1.280	0.783
Clay	< 0.5 m	B11	0.00	0.60	2.43	1.111	2.617
	> 0.5 m	O12	0.00	0.56	0.95	1.159	1.212
Loam	< 0.5 m	B14	0.01	0.42	0.51	1.305	0.638
	> 0.5 m	O15	0.01	0.41	1.71	1.298	1.136
Peat	> 0.5 m	B16	0.00	0.63	1.34	1.320	1.051
	< 0.5 m	O16	0.79	0.00	1.03	1.376	0.226
glacial	< 0.5 m	B1	0.43	0.01	2.49	1.507	0.478
till	> 0.5 m	O6	0.41	0.00	2.91	1.152	1.271

[a] refers to the 'Winand Staring Soil Series'

[b] taken from the old Soil Series, as these agree better to field measurements (Tiktak and Bouten, 1985; Tiktak, 1984; Bouten, 1992).

Parameter values were selected from the 'Winand Staring soil series' in which parameter values are given for 18 texture classes (Wösten *et al.*, 1994; Wösten *et al.*, 1995), and are listed in table 6. For each major soil type, the set of parameters associated with the dominant texture class within each major soil type was considered.

The pore volume, ϕ ($m^3\ m^{-3}$) was calculated from the saturated soil water content by:

$$\phi = 1.198\,\theta_s \tag{27}$$

The factor 1.198 was included to account for the effect of residual air during soil wetting (Dracos, 1991). It corresponds to the average fraction of residual air (0.198) found by Freijer (1995).

A continuous pedotransfer approach was used to relate the bulk density, ρ_b (kg m^{-3}), to the organic matter content (Bollen *et al.*, 1995):

$$\rho_b = (\ 1799.7 + 1236.0\,f_{om} - 2912.0 \cdot \sqrt{f_{om}}\,) \qquad (r^2 = 0.91) \tag{28}$$

The density of the soil solid phase, ρ_s (kg m^{-3}) was calculated according to:

$$\rho_s = \frac{\rho_b}{(\ 1 - \phi\ )} \tag{29}$$

The air-filled porosity at the air-entry value, ε_o (Eq. (14)), was calculated from ϕ-θ_α, where θ_α is the water content at a pressure head equal to the air-entry value (-1/α). Parameter *a* (Eq. (14)) was calculated from measured diffusion characteristics (Freijer, 1995), and was set equal to 1 for sand, loam and peat soils, and 0.5 for sandy-clay, clay, and boulder-clay soils.

3.1.3 Spatially-constant parameters

Crop properties

The reduction function for water uptake, *f(h)* (Eq. (2)), was set at 1 (no reduction) for $h > -0.5$ m, and decreased linearly to 0 between $h = -0.5$ m and $h = 0.8$ m (wilting point). These values were based on a field study for maize (Boesten and Van der Linden, 1991).

Soil properties

The parameter β (Eq. (5)) describing the reduction of evaporation due to drying of the top layer was estimated to be 2 $mm^{1/2}$ (Boesten and Stroosnijder, 1986). The dispersion length L_{dis} (Eq. (10)) was set at 0.05 m for all soil types, which is in the range of values found by van Ommen *et al.* (1989). The tortuosity factor for diffusion λ (Eq. (11)) was assumed to be a function of the water content as described by Leistra (1978).

Pesticide properties and application practices

All pesticides were applied on May 25 (spring application) or November 1 (autumn application) at a rate of 1 kg ha^{-1}. Table 7 shows the application type, the fraction of pesticide applied in spring (f_s), loss during application (f_a), the degradation half-life (DT_{50}), the coefficient for distributing the pesticide over organic matter and water (K_{om}), the coefficient for distribution over the gas and water phases (K_H), and the formation fractions of metabolites (f_f) for a total number of 21 mobile pesticides. Pesticide losses during application include interception by the vegetation and drift, and were derived from Jager *et al.*, 1992. The Freundlich exponent, *1/n*, was set equal to 0.9, which is the average of values reported by Calvet *et al.* (1980). The diffusion coefficient of the pesticide in water, D_o, was estimated to be 40 mm^2 d^{-1}. This is a normal value for pesticide molecules with a relative molecular mass of about 200 as estimated using methods described by Reid and Sherwood (1966). The effective diffusion coefficient of pesticide in free air ($D_{eff,Fi}$, Eq. (15)) was estimated at 0.4 m^2 d^{-1} (Freijer *et al.*, 1996). The parameter γ in Eq. (20) was 0.08 K^{-1}. This is the average of some 50 experiments with a range of pesticides and soils as reviewed by Boesten (1986) and approximately corresponds with a molar energy of activation in the Arrhenius equation of 55 kJ mol^{-1}. The parameter B in Eq. (21) was 0.25, which is the average of values found in 40 experiments with a range of pesticides and soils (Boesten and van der Linden, 1991)[1].The factor f_z in Eq. (19) was 1 in the top 0.3 m, and it decreased linearly to 0.9 at 0.5 m; between 0.5 and 1.0 m it decreased linearly to zero (Boesten and van der Linden, 1991). The transpiration stream concentration factor for pesticide uptake, f_{uc}, in Eq. (22) was 0.5, which is the average of values reported in Briggs *et al.*, 1982.

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[1] Parameter B was originally obtained for the relationship $f_\theta = (\theta/\theta ref)^B$. It has been converted to the notation described in equation 21 using the physical characteristics for loamy fine sand (B2).

TABLE 7

Application type, fraction of total dose applied in spring (f_s), loss during application (f_a), and chemical properties[a] of 21 mobile pesticides[b]. Pesticide properties were taken from Linders *et al.* (1993), and data on application losses from Jager *et al.*, 1992.

pesticide	application type	f_s	f_a S[g]	f_a A[g]	f_f	DT_{50}	K_{om}	K_H[f]
		(-)	(-)		(-)	(d)	(L kg^{-1})	(m^3 m^3)
aldicarb	ploughing[c]	0.83	0.0	0.0	-	2.4	48.0	0.0
> aldicarb-sulfoxide	daughter of aldicarb	-	-	-	0.76	22.0	1.4	0.0
> aldicarb-sulphone	daughter of sulphoxide	-	-	-	0.66	48.0	0.5	0.0
atrazine	surface application[d]	1.00	0.2	-	-	50.0	70.0	0.0
> desethyl-atrazine	daughter of atrazine	-	-	-	0.21	45.0	18.0	0.0
bentazone	surface application	0.93	0.2	0.5	-	16.0	0.4	0.0
captan	surface application	1.00	0.2	-	-	1.0	75.0	0.0
carbendazim	surface application	0.99	0.5	0.5	-	52.0	76.0	0.0
carbofuran	surface application	0.99	0.0	0.5	-	30.0	11.0	0.0
chloridazon	surface application	1.00	0.2	-	-	31.0	64.0	0.0
cis-1,3-DCP	injection[e]	0.05	0.0	0.0	-	7.84	15.0	0.056
DNOC	surface application	1.00	0.2	-	-	8.5	20.6	0.0
chlorothalonile	surface application	0.99	0.5	0.5	-	10.0	5031.0	0.0
> isophtalonitrile	daughter of chlorothalonile	-	-	-	0.35	387.0	14.0	0.0
dicamba	surface application	1.00	0.3	-	-	48.0	0.0	0.0
lenacil	surface application	1.00	0.0	-	-	179.0	20.0	0.0
mecoprop-p	surface application	0.30	0.5	0.5	-	11.0	0.0	0.0
metalaxyl	surface application	0.94	0.5	0.5	-	42.0	27.0	0.0
> methoxyacetylalanine	daughter of metalaxyl	-	-	-	0.46	58.0	22.0	0.0
metam-sodium	ploughing	0.05	0.0	0.0	-	<0.01	228.0	0.0
> methylisothiocyanate	daughter of metam-sodium	-	-	-	0.48	6.0	3.0	0.0068
metholachloor	surface application	1.00	0.5	-	-	101.0	103.0	0.0
oxamyl	surface application	0.35	0.0	0.0	-	18.0	2.0	0.0
pendimethalin	surface application	1.00	0.0	-	-	171.0	111.0	0.0
pyridaat	surface application	1.00	0.2	-	-	38.0	7.0	0.0

[a] f_f is formation constant of metabolite; DT_{50} is degradation half-life; K_{om} is coefficient for partitioning over organic matter and water; K_H is coefficient for partitioning over water and gas phases. Some of the pesticide properties are under reconsideration, and therefore do not necessarily represent the latest view.

[b] Data are available for a total number of 350 pesticides. However, we did not carry out a simulation for those pesticides that were expected to give a total leaching of less than 100 kg for the Netherlands.

[c] Surface application, followed by instantaneous mixing of the upper 15 cm of the soil profile.

[d] Surface application, followed by instantaneous mixing of the upper 5 cm of the soil profile.

[e] Injection at 17.5 cm depth.

[f] 0.0 indicates $K_H < 10^{-5}$.

[g] S = spring application; A = autumn application

4 VULNERABILITY TO PESTICIDE LEACHING

A first step in obtaining spatial patterns of pesticide leaching is the assessment of the vulnerability of geographic locations to pesticide leaching, using a standard dose of 1 kg ha^{-1} (section 2.1). This assessment has been carried out for all pesticides listed in table 7. Results are described in this chapter. Section 4.1 discusses the sensitivity of pesticide leaching to the independent spatially-distributed parameters, section 4.2 shows vulnerability maps, and in section 4.3 somes uncertainties are discussed.

The discussion in this chapter is focused onto four pesticides with different properties, i.e. atrazine (moderately mobile; moderately degradable), bentazone (very mobile; fairly degradable), isophtalonitrile (daughter of chlorothalonil, fairly mobile; persistent), and cis-1,3-DCP (fairly mobile; fairly degradable; volatile). The application schedule was chosen in correspondence with the normal application schedule for each individual pesticide, i.e. spring application for atrazine, bentazone, and chlorothalonile, and autumn application for cis-1,3-DCP. The end date for all simulations was set at the time that 0.01% of the applied dose was still present in the soil column. Using the procedure described above, the number of mega-plots for which the model had to be run could be effectively reduced from 93000 (which is the total number of relevant 500×500 m^2 grid-cells in the Netherlands) to 897. For all these mega-plots, the execution time was approximately 2-4 hours (HP workstation) for each pesticide considered.

4.1 Sensitivity of leaching to independent spatial parameters

Table 8 shows the relative importance of transformation, uptake by plant roots, volatilization, and leaching for 18 combinations of basic spatially-distributed parameters, and was obtained by varying one of the distinguished basic spatially-distributed parameters, while keeping all other parameters constant. Figure 8 shows the average concentration of the four pesticides in the soil solution between 1 and 2 m depth for the same combinations. Notice that some combinations of independent spatially-distributed parameter are not realistic. They were added to show the effect of combining individual spatially-distributed parameters only. For example, peat soils with an average organic matter content of 0.4% are non existing. Figure 8 and table 8 show that transformation, uptake, volatilization, and leaching are strongly dependent on pesticide properties. Boesten and van der Linden (1991) found that changing K_{om} or DT_{50} by a factor 2 usually changes the amount leached by roughly a factor 10.

Soil type

Soil type (i.e. soil physical characteristics) has a clear effect on both the magnitude of the maximum concentration, and the time that this concentration was reached (Figure 8), caused by differences in the water holding capacity of the soils. Notice that differences in the magnitude of the concentration are highest for mobile pesticides, such as bentazone. The fraction of pesticide taken up is highest in sandy soils and lowest in peat soils (table 8). This effect is caused by differences in the soil water content (highest in peat soils), which in turn causes differences in the aqueous concentrations after application (lowest in peat soils), and root uptake fluxes (Eq. (22)). At the same time, the fraction of pesticide transformed is highest in peat soils. This difference is explained by higher residence times in peat soils. The overall result of these two processes is that leaching from peat soils is lowest, whereas the opposite is true for sandy soils (table 8). Notice that the relative importance of loss pathways is less sensitive to soil physical characteristics (dependent on soil type) for atrazine. This confirms findings in an earlier sensitivity analysis (Tiktak *et al.*, 1994b), which showed that the fraction of pesticide leached from the upper meter is most sensitive to sorption parameters with higher values of K_{om}. Soil type has a tremendous effect on volatilization of cis-1,3-DCP. In sandy soils, soil water pressure heads were usually below the air entry value during the first 14 days after application, while pressure heads were above the air entry value in other soils. Thus, in heavier textured soils, transport by Fickian diffusion is blocked and volatilization negligible (Eqn. (13) and (14)). It should be noted that these differences are less pronounced when the pesticide is applied in spring (data not shown). Notice that the effect on leaching of cis-1,3-DCP is less extreme. This corresponds to findings by Freijer *et al.* (1996) who found that when the fraction volatilized decreased, the remainder usually transformed (competition between transformation and volatilization).

Crop type

The most important parameters for the fate of pesticides in relation to crop-type are the maximum root penetration depth, and crop phenology (table 5). Pesticide uptake is highest for grass (table 8). This is the result of the shallow root depth, causing high water uptake fluxes from the upper soil layer, close to the point of pesticide application. The overall effect is that leaching from grassland is lowest. Notice that the effects of crop type are most pronounced for mobile pesticides (relatively high aqueous concentration). 1,3-DCP is not or hardly taken up by the crop, as it is applied in autumn.

Organic matter content

Generally, the fraction of pesticide leached from the upper meter decreases with increasing organic matter content. The same is true for the uptake fraction. Table 8 shows only one exception to this general rule: the fraction of chlorothalonile leached from the soil column is highest for the second organic matter category. This is the result of calculated high uptake rates for soils with very low organic matter contents, which agrees with findings of Leistra and Dekkers (1976) who found very high uptake rates when $K_{om} f_{om} \approx 0$. The table shows that the leaching potential of atrazine depends almost entirely on organic matter content, confirming results of the earlier sensitivity analysis as described before.

Groundwater level

Table 8 shows that the fraction leached from the upper meter is highest in cases with deep groundwater tables, where upward water flow is negligible. With deep groundwater tables, soil water contents in the uppermost soil layer are relatively low. As a results, aqueous concentrations of pesticide directly after application are high, causing high uptake fractions (see discussion above). A contrasting effect of these low soil water contents is reduction of pesticide transformation (Eq. (21)). For the selected pesticides the effect on transformation is somewhat greater than the effect on uptake, resulting in higher leaching levels for deep groundwater tables. For atrazine there is hardly any effect on transformation. This pesticide will be retained in the upper soil layers for a longer time where it will be subject to transformation when soil water contents increase later on in the season. Figure 8 clearly shows the longer breakthrough time for atrazine, compared to chlorothalonile and bentazone. Differences in the leaching fraction are most pronounced for 1,3-DCP. This is caused by Fickian diffusion of this pesticide, resulting in enhanced transport in cases with deep groundwater tables to both the atmosphere, and the groundwater.

Annual precipitation

Annual precipitation amounts have only a minor effect on model outputs (Table 8 and Figure 8). It may be questioned whether this is primarily caused by the assumption that the temporal dynamics of rainfall is constant across the country. However, even in the Netherlands where differences in altitude are in the order of tens of meters, a clear orographic effect on precipitation is found, and it is generally acknowledged that the seasonal variation of rainfall is different for regions with higher altitude (more thunderstorms in summer). To check the effect of precipitation distribution during the year, 30 simulations were done with different distributions of rainfall over the season, but with equal amounts of annual precipitation. For each individual model run, daily weather conditions were derived from the 1961-1990 climatic record from ‘De Bilt’ by the equation

$$P_d^{\prime} = P_d \frac{\overline{P_a}}{P_a} \tag{30}$$

where P_d' (m d^{-1}) is corrected daily precipitation, P_d (m d^{-1}) is measured daily precipitation, $\overline{P_a}$ (m a^{-1}) is long-term average annual precipitation, and P_a (m a^{-1}) annual precipitation for an individual year. As the variation of rainfall distribution across the country rarely exceeds the variation between individual years, these simulations provide a worst-case estimate of the uncertainty due to different seasonal distributions of rainfall. Figure 9 summarizes the results of the simulations as a cumulative frequency distribution function. The figure shows that the variation of the maximum concentration in the 1-2 m soil layer, expressed as a fraction of the long-term average value is highest for the mobile pesticide bentazone, and lowest for the pesticide with the highest disappearance half-life, chlorothalonile. Generally, predicted concentrations are highest for those model-runs with high precipitation within one month after pesticide application. This phenomenon can be explained as follows: When it rains within a few days after pesticide application, a mobile pesticide will be quickly transported to greater depths in the soil profile, where it is subject to slower degradation. This causes both high leaching fractions, and high concentrations of pesticide in the upper groundwater. This effect will be negligible for pesticides with long half-lives, such as hydroxy-chlorothalonile. The behaviour of atrazine is in between.

TABLE 8.A

Cumulative fluxes of pesticide (% of applied dose) at the end of the simulations for 18[§] combinations of basic spatially-distributed parameters. Both atrazin and bentazone were applied on May 25 (spring application).

soil type	land use	f_{om}[†] (%)	GWC[‡]	P (mm)	atrazine				bentazone			
					fr_l[¶] (%)	fr_{vol}	fr_{tr}	fr_{up}	fr_l[¶] (%)	fr_{vol}	fr_{tr}	fr_{up}
Effect of soil type												
loam-poor sand	maize	1.6	mod. deep	808	1.2	0.0	92.9	5.9	2.6	0.0	76.0	21.4
loamy-sand	maize	1.6	mod. deep	808	1.2	0.0	92.9	5.9	2.3	0.0	76.7	21.0
sandy-clay	maize	1.6	mod. deep	808	1.0	0.0	93.2	5.8	0.8	0.0	81.5	17.7
silty-loam	maize	1.6	mod. deep	808	1.1	0.0	93.1	5.8	0.8	0.0	81.7	17.5
clay	maize	1.6	mod. deep	808	0.7	0.0	93.7	5.6	0.3	0.0	85.1	14.5
peat	maize	1.6	mod. deep	808	0.5	0.0	93.9	5.6	0.2	0.0	85.2	14.6
Effect of crop type												
loamy-sand	grass	1.6	mod. deep	808	0.8	0.0	89.5	9.7	3.2	0.0	68.6	28.3
loamy-sand	maize	1.6	mod. deep	808	1.2	0.0	92.9	5.9	2.3	0.0	76.7	21.0
Effect of organic matter content												
loamy-sand	maize	0.4	mod. deep	808	7.8	0.0	76.7	15.5	2.5	0.0	75.9	21.6
loamy-sand	maize	1.2	mod. deep	808	1.9	0.0	91.0	7.1	2.4	0.0	76.5	21.1
loamy-sand	maize	1.6	mod. deep	808	1.2	0.0	92.9	5.9	2.3	0.0	76.7	21.0
loamy-sand	maize	2.1	mod. deep	808	0.7	0.0	94.4	4.9	2.2	0.0	76.9	20.9
loamy-sand	maize	6.0	mod. deep	808	0.0	0.0	97.6	2.4	1.9	0.0	78.3	19.8
Effect of Groundwater Class												
loamy-sand	maize	1.6	ver. shal.	808	1.1	0.0	93.2	5.7	1.1	0.0	78.9	20.0
loamy-sand	maize	1.6	fai. shal.	808	1.1	0.0	93.2	5.7	1.2	0.0	78.1	20.7
loamy-sand	maize	1.6	mod. deep	808	1.2	0.0	92.9	5.9	2.3	0.0	76.7	21.0
loamy-sand	maize	1.6	fai. deep	808	1.4	0.0	92.7	5.9	2.3	0.0	74.3	23.4
loamy-sand	maize	1.6	deep	808	1.7	0.0	92.1	6.2	2.2	0.0	69.2	28.6
Effect of precipitation												
loamy-sand	maize	1.6	mod. deep	748	0.9	0.0	93.2	5.9	1.4	0.0	76.8	21.8
loamy-sand	maize	1.6	mod. deep	779	1.0	0.0	93.1	5.9	1.8	0.0	76.8	21.4
loamy-sand	maize	1.6	mod. deep	808	1.2	0.0	92.9	5.9	2.3	0.0	76.7	21.0
loamy-sand	maize	1.6	mod. deep	819	1.5	0.0	92.6	5.9	3.0	0.0	76.4	20.6

§) The total number of lines in the table is 22, as the combination loamy-sand-maize-1.6-moderately-deep-808 is listed in all series.

†) f_{om} (%) is average organic matter content of the upper meter of the soil.

‡) GWC is groundwater-depth-class.

¶) fr_l (%) is fraction leached from the upper meter of the soil column, fr_{vol} (%) is fraction volatilized, fr_{tr} (%) is fraction transformed, and fr_{up} (%) is fraction taken up by plants.

TABLE 8.B

Cumulative fluxes of pesticide (% of applied dose) at the end of the simulations for 18§ combinations of basic spatially-distributed parameters. Chlorothalonil was applied on May 25 (spring application), and cis-1,3-DCP on November 1 (autumn application).

soil type	land use	f_{om}† (%)	GWC‡	P (mm)	hydroxy-chlorothalonile				cis-1,3-DCP			
					fr_l¶ (%)	fr_{vol}	fr_{tr}	fr_{up}	fr_l¶ (%)	fr_{vol}	fr_{tr}	fr_{up}
Effect of soil type												
loam-poor sand	maize	1.6	mod. deep	808	18.2	0.0	73.2	8.6	2.8	32.0	65.2	0.0
loamy-sand	maize	1.6	mod. deep	808	18.1	0.0	73.3	8.6	2.2	33.1	64.7	0.0
sandy-clay	maize	1.6	mod. deep	808	17.5	0.0	74.3	8.2	0.5	0.0	99.5	0.0
silty-loam	maize	1.6	mod. deep	808	17.7	0.0	74.1	8.2	0.6	0.0	99.4	0.0
clay	maize	1.6	mod. deep	808	16.5	0.0	75.7	7.8	0.2	0.0	99.8	0.0
peat	maize	1.6	mod. deep	808	16.0	0.0	76.2	7.8	0.1	0.0	99.9	0.0
Effect of crop type												
loamy-sand	grass	1.6	mod. deep	808	15.6	0.0	73.6	10.8	1.7	33.4	64.3	0.6
loamy-sand	maize	1.6	mod. deep	808	18.1	0.0	73.3	8.6	2.2	33.1	64.7	0.0
Effect of organic matter content												
loamy-sand	maize	0.4	mod. deep	808	17.1	0.0	69.6	13.3	4.6	48.6	46.8	0.0
loamy-sand	maize	1.2	mod. deep	808	18.2	0.0	72.3	9.5	2.7	36.5	60.8	0.0
loamy-sand	maize	1.6	mod. deep	808	18.1	0.0	73.3	8.6	2.2	33.1	64.7	0.0
loamy-sand	maize	2.1	mod. deep	808	17.6	0.0	74.6	7.8	1.6	29.7	68.7	0.0
loamy-sand	maize	6.0	mod. deep	808	12.5	0.0	81.7	5.8	0.2	17.4	82.4	0.0
Effect of Groundwater Class												
loamy-sand	maize	1.6	ver. shal.	808	17.8	0.0	73.8	8.4	0.5	6.8	92.7	0.0
loamy-sand	maize	1.6	fai. shal.	808	17.9	0.0	73.7	8.4	0.7	16.1	83.2	0.0
loamy-sand	maize	1.6	mod. deep	808	18.1	0.0	73.3	8.6	2.2	33.1	64.7	0.0
loamy-sand	maize	1.6	fai. deep	808	18.4	0.0	72.9	8.6	3.6	34.7	61.7	0.0
loamy-sand	maize	1.6	deep	808	19.1	0.0	72.4	8.5	5.2	36.4	58.4	0.0
Effect of precipitation												
loamy-sand	maize	1.6	mod. deep	748	16.9	0.0	74.1	9.0	1.7	33.9	64.4	0.0
loamy-sand	maize	1.6	mod. deep	779	17.6	0.0	73.7	8.7	1.9	33.4	64.7	0.0
loamy-sand	maize	1.6	mod. deep	808	18.1	0.0	73.3	8.6	2.2	33.1	64.7	0.0
loamy-sand	maize	1.6	mod. deep	819	18.7	0.0	72.9	8.4	2.7	32.6	65.0	0.0

§) The total number of lines in the table is 22, as the combination loamy-sand-maize-1.6-moderately-deep-808 is listed in all series.

†) f_{om} (%) is average organic matter content of the upper meter of the soil.

‡) GWC is groundwater-depth-class.

¶) fr_l (%) is fraction leached from the upper meter of the soil column, fr_{vol} (%) is fraction volatilized, fr_{tr} (%) is fraction transformed, and fr_{up} (%) is fraction taken up by plants.

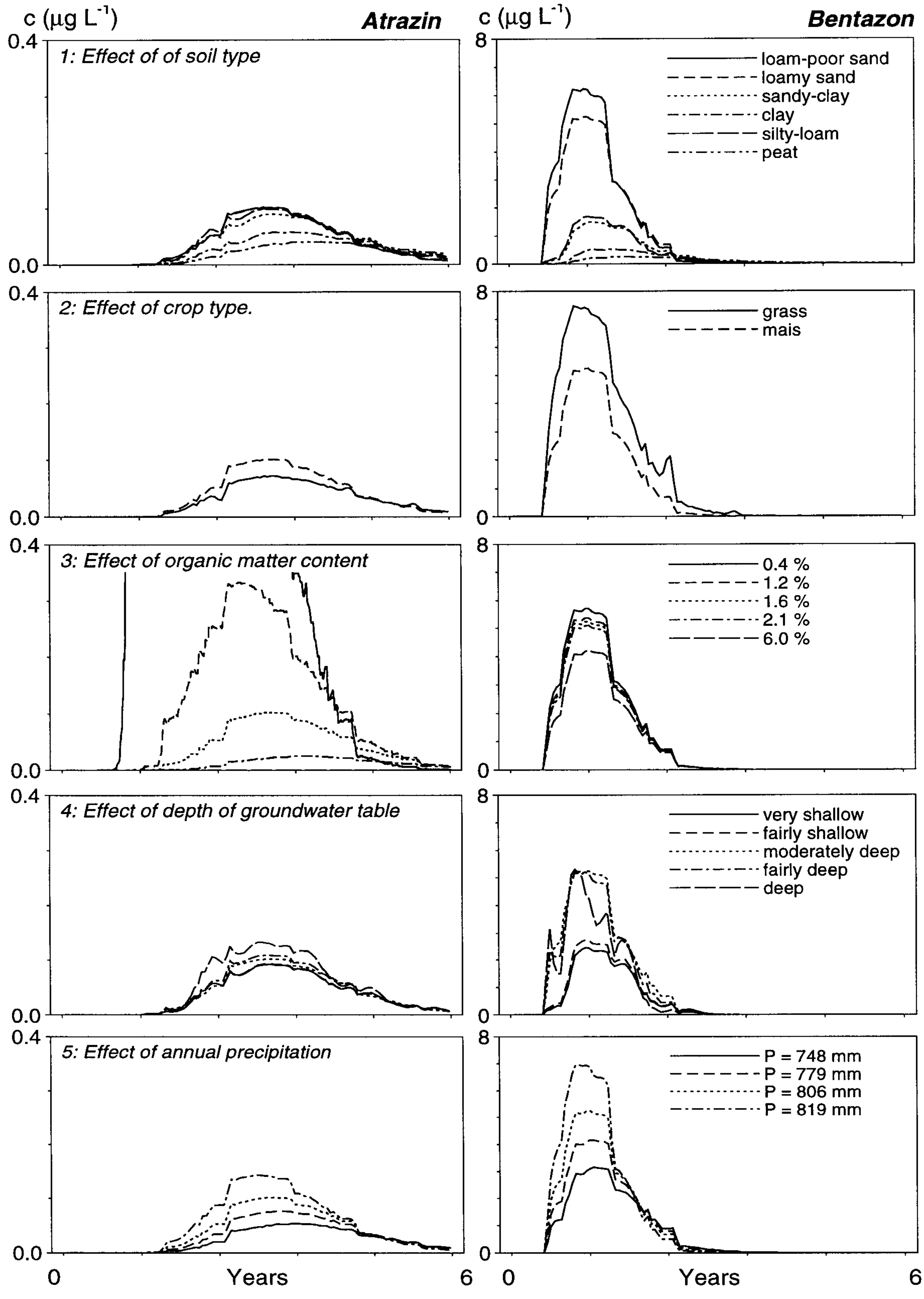


Figure 8a.

Sensitivity of the average concentration of atrazine and bentazon in the soil solution between 1 and 2 m depth to soil type, crop-type, organic-matter-content, groundwater depth and annual precipitation.

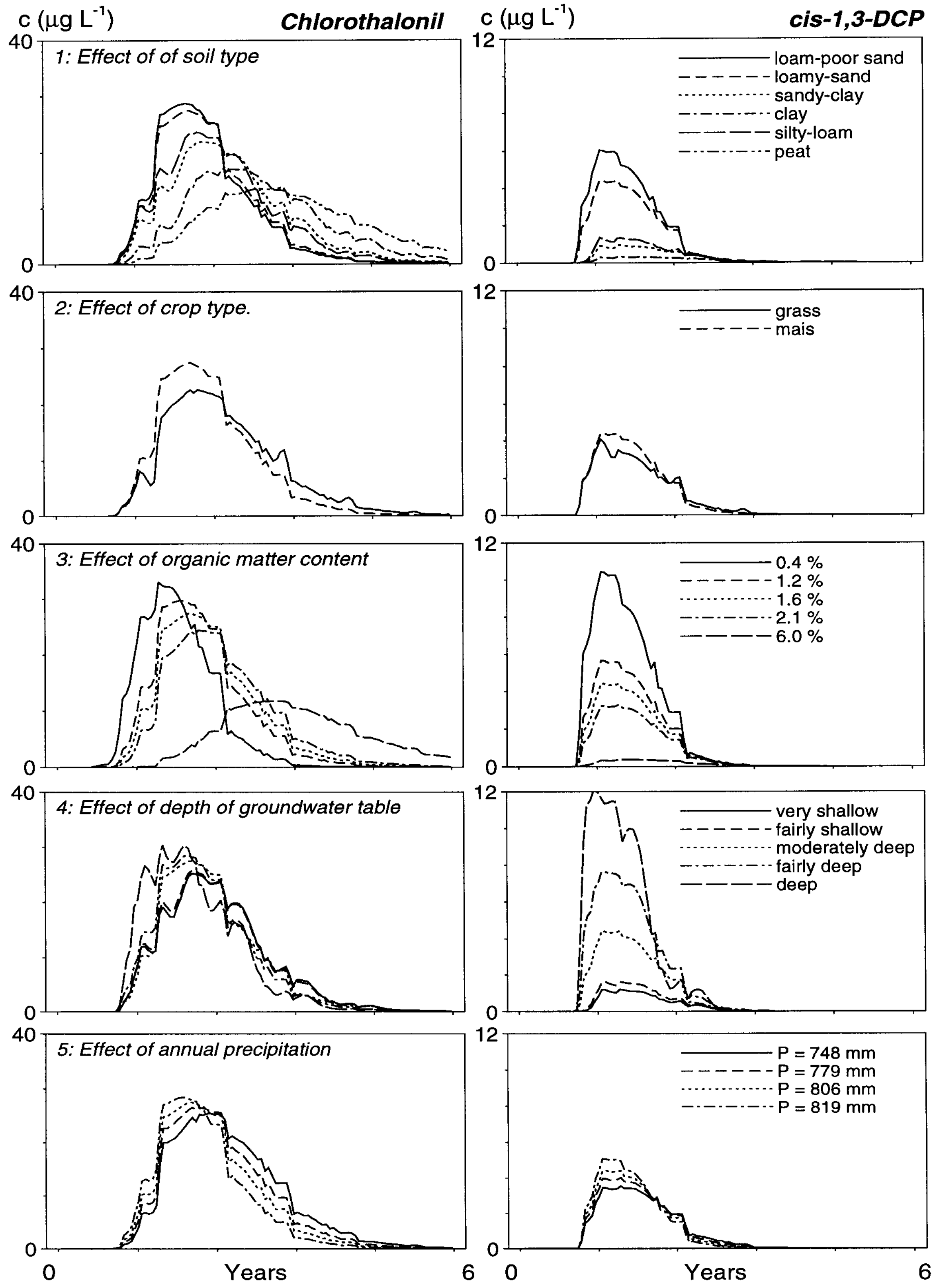


Figure 8b.

Sensitivity of the average concentration of chlorothalonile and cis-1,3-DCP in the soil solution between 1 and 2 m depth to soil type, crop-type, organic-matter-content, groundwater depth and annual precipitation.

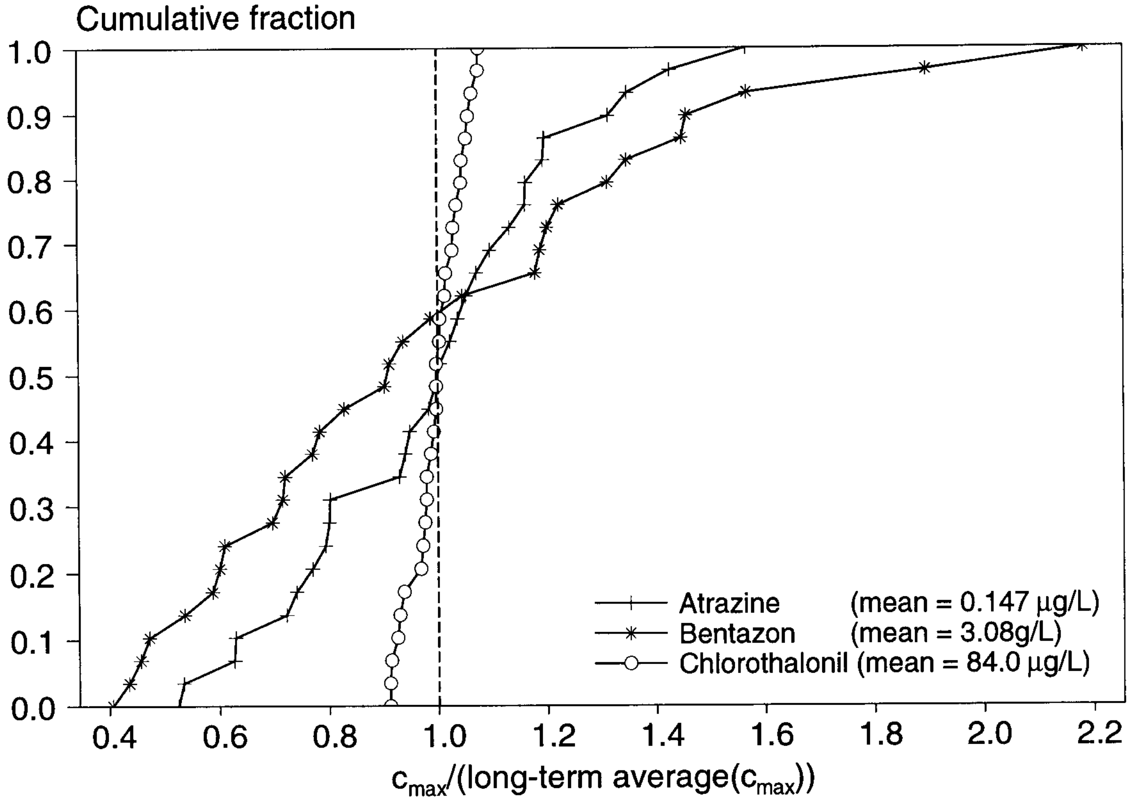
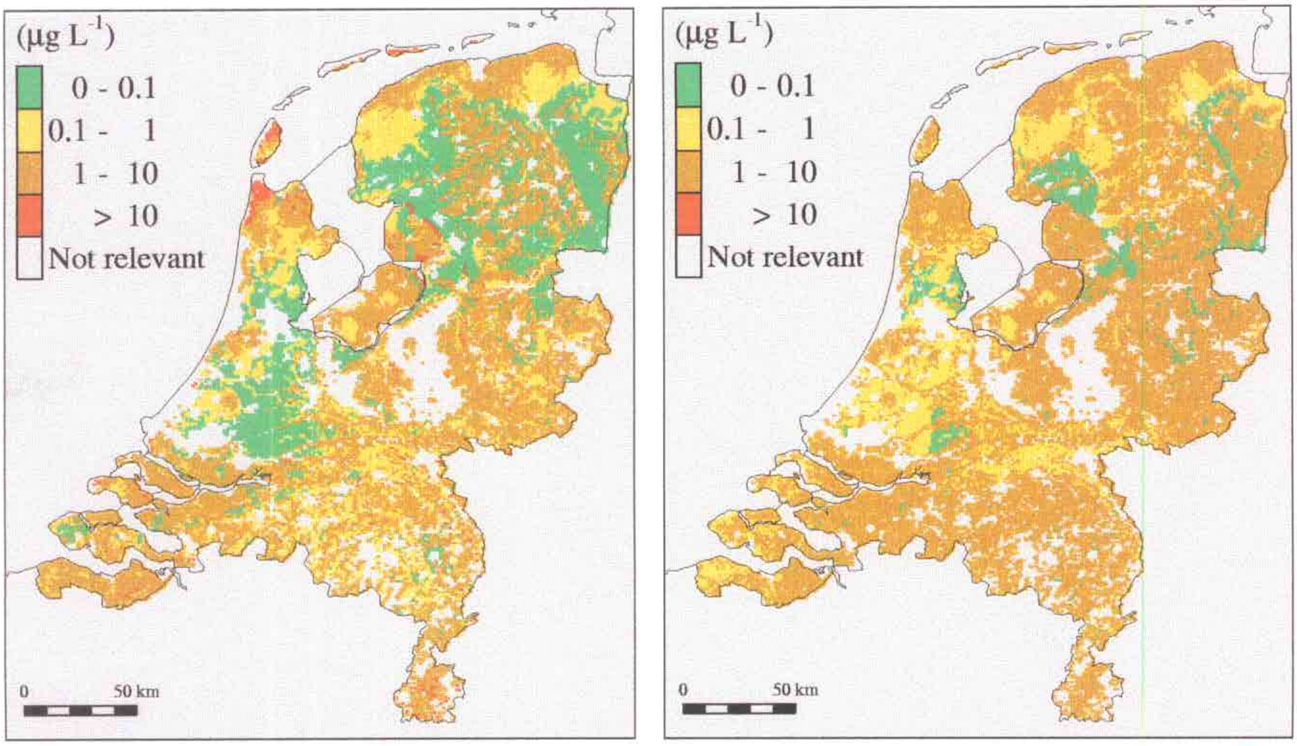


Figure 9.

Cumulative distribution functions of the maximum concentration of pesticide in the 1-2 m soil layer, scaled to the long-term average maximum concentration. The figure shows the effect of different seasonal patterns of precipitation.

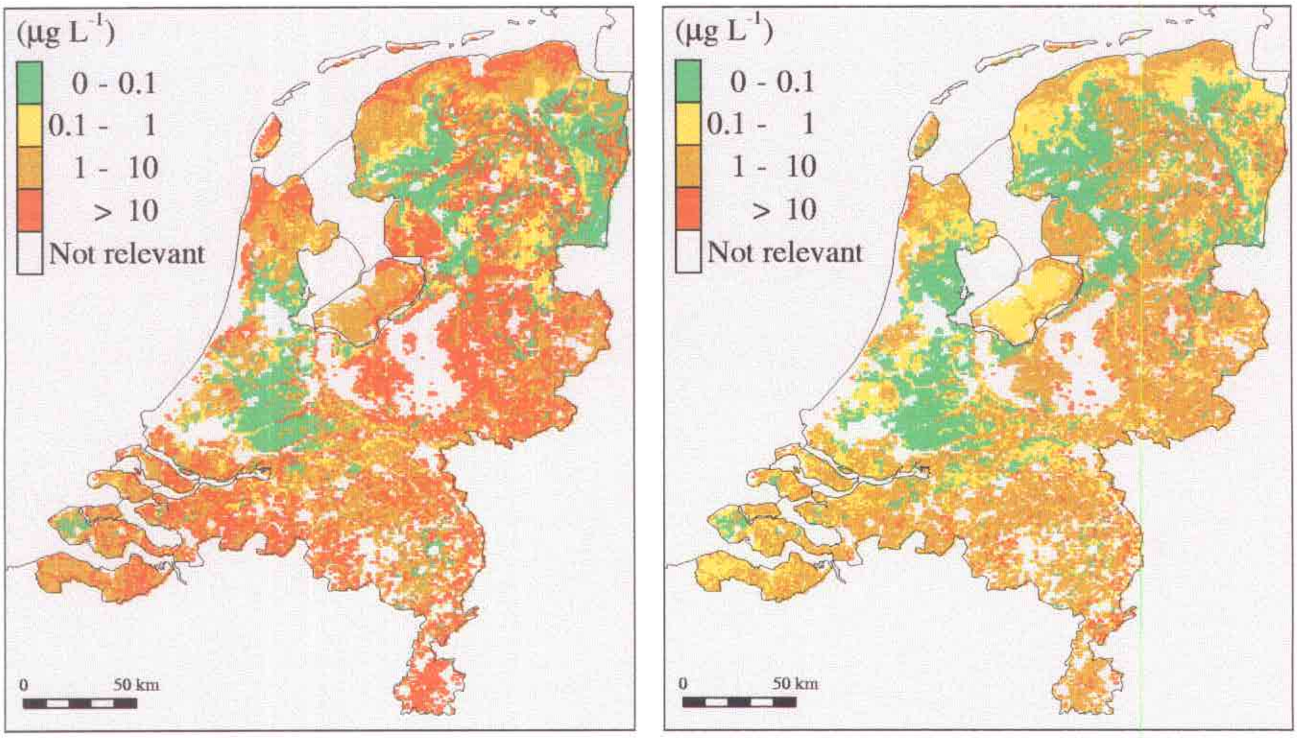
4.2 Vulnerability maps

Figure 10 shows the simulated maximum aqueous concentrations of atrazine, bentazone, chlorothalonile, and cis-1,3-DCP in the 1-2 m soil-layer. For the generation of these maps, the standard scenario as described before has been used. The point in time associated with the maximum concentration depends on both pesticide properties and soil properties, and ranges from 400-1200 days (see also Figure 8).



Atrazine (spring application)

Bentazone (spring application)



Chlorothalonile (spring application)

Dichloropropene (autumn application)

Figure 10

Average maximum concentration of pesticide in the 1-2 m soil layer, using a dose of 1 kg ha $^{-1}$. This map can be used to classify the vulnerability of geographic locations relative to each other. Maps showing the leaching with the actual dose are shown in chapter 5.

Comparison with basic spatially-distributed parameters

Table 9 shows the linear correlation coefficients amongst each of the six basic spatially-distributed parameters on the one hand, and the maximum concentration in the upper groundwater on the other hand. Each pesticide is most strongly correlated with a different basic spatially-distributed parameter. For example, the maximum concentration of atrazine correlates strongly with organic matter content, the map of the maximum bentazone concentration shows most resemblance with the soil type map, and the concentration of dichloropropene correlates most strongly with groundwater depth class. The table also shows that precipitation, evapotranspiration and crop-type do not not or hardly correlate with the maximum concentration. All these findings are entirely in line with results in section 4.1. Summarizing it can be stated that:

- moderately mobile and moderately degradable pesticides (e.g. atrazine) are highly dependent upon the organic matter content, which is a parameter relevant to the sorption of the pesticide.
- the concentration of mobile pesticides with moderate to high half-lives (e.g. bentazone and chlorothalonile) shows strong correlation with the soil type map (soil physical conditions).
- the concentration of volatile pesticides is highly dependent upon soil type and groundwater level.

TABLE 9

Square of the linear correlation coefficients, r^2, amongst each of the six basic spatially-distributed variables on the one hand, and the maximum concentration on the other hand. All regression coefficients are significant at the 0.01 probability level.

	r^2			
Basic variable	atrazine	bentazone	chlorothalonile	cis-1,3-DCP
Organic matter content	0.941	0.639	0.602	0.821
Soil type	0.600	0.897	0.799	0.601
Groundwater Depth Class	0.421	0.335	0.301	0.870
Land-use	0.066	0.037	0.078	0.021
Precipitation	0.051	0.061	0.053	0.135
Reference evapotranspiration	0.023	0.041	0.035	0.017

Visual comparison of Figure 7 and Figure 10 shows that despite the differences between the four pesticides, concentration levels are lowest under peat soils, and concentrations are at their maximum under sandy and loamy soils with low organic matter contents (loess and dune soils). Notice that contrary to the fact that the leaching of bentazone is virtually independent of organic matter content (Figure 8), the concentration of bentazone is highly correlated with organic matter content map. This is caused by cross-correlations between the soil texture and organic matter content maps. This implies that conclusions about the underlying processes cannot be made by simply comparing pesticide leaching maps with a map of one single model input.

4.3 Some remarks on uncertainty

The output of any mathematical model is highly dependent upon the underlying model concepts, and assumptions about input parameters (Janssen and Heuberger, 1995; Leijnse and Hassanizadeh, 1994). In regional model applications, both the spatial variability of model parameters such as soil texture and organic matter content, and temporal variation of boundary conditions such as rainfall distribution affect the predictions. As both the concepts, and the parameters are incompletely known in natural systems, regional scale model predictions will always have a high degree of uncertainty, as shown, for example, by Loague *et al.* (1989).

To evaluate the effects of the hypothesized relationships and assumptions in the model (transformation dependence on water content, temperature and depth-in-soil; equilibrium sorption; no preferential flow; no surface runoff), field tests are indispensable, as indicated by Wagenet and Rao (1985) and Boesten and van der Linden (1991). For validation of regional scale models, it is necessary to have the model applied under a broad range of conditions. Recently, field tests of the underlying model were carried out in sandy soils (Boekhold *et al.*, 1993; Van den Bosch and Boesten, 1994). In the near future, the model will be applied to various field data-sets, and results will be compared to those generated by models including preferential flow (Jarvis, 1991). The lack of field-tests in fine-textured soils implies that currently the uncertainty about model concepts is higher in fine-textured soils than in sandy soils. However, some regional scale monitoring data (Leistra and Boesten, 1989; Kohsiek, 1991) confirm the general patterns predicted by the model. They found pesticides in groundwater only in areas that we have classified vulnerable.

The effect of uncertain model parameters is often assessed by performing Monte-Carlo simulations taking into account cross-correlations between input variables (Heuberger and Janssen, 1993; Loague *et al.*, 1989; Tiktak *et al.*, 1994b). A disadvantage of the Monte-Carlo technique for complex regional scale models is the large number of model runs that must be carried out. In this paper, the effect of uncertainty of two important basic spatially-distributed model parameters is assessed by systematically changing one of these parameters, while keeping all other parameters constant. The effect of spatial variability of organic matter content within each mega-plot was assessed by calculating vulnerability maps using the minimum, mean, and maximum organic matter contents for each given 500×500 m^2 grid-cell. The minimum and maximum contents were determined by looking up within each grid-cell the soil type with the lowest and highest organic matter content, the mean was calculated using an area weighted averaging procedure as described in the section on model inputs. The influence of temporal variation of precipitation was assessed by calculating 30 vulnerability maps for both pesticides, where each map is associated with weather conditions from a different year in the period 1961-1990.

Results are presented as cumulative distribution functions of the maps of the maximum concentrations of atrazine and bentazone (Figure 11). The figure shows that variability of organic matter content has a large effect on atrazine leaching, but also that the effect on bentazone leaching is negligible. Temporal variability of weather conditions, on the other hand, has a large effect on bentazone leaching. These findings are entirely in line with results from preceding sections, which showed high sensitivity to seasonal variability of weather conditions, but low sensitivity to annual rainfall amounts. Notice that the frequency distribution function of the atrazine leaching map associated with average organic matter contents is close to the minimum value. This supports the well-known fact that simulations based on average soil properties (in this case organic matter content) may significantly underestimate the average leaching.

These two examples demonstrate that the fate of pesticides is strongly dependent upon pesticide properties. They also demonstrate that general conclusions on the fate of pesticides in the soil cannot be drawn on the basis of results for a single pesticide, or a single parameter.

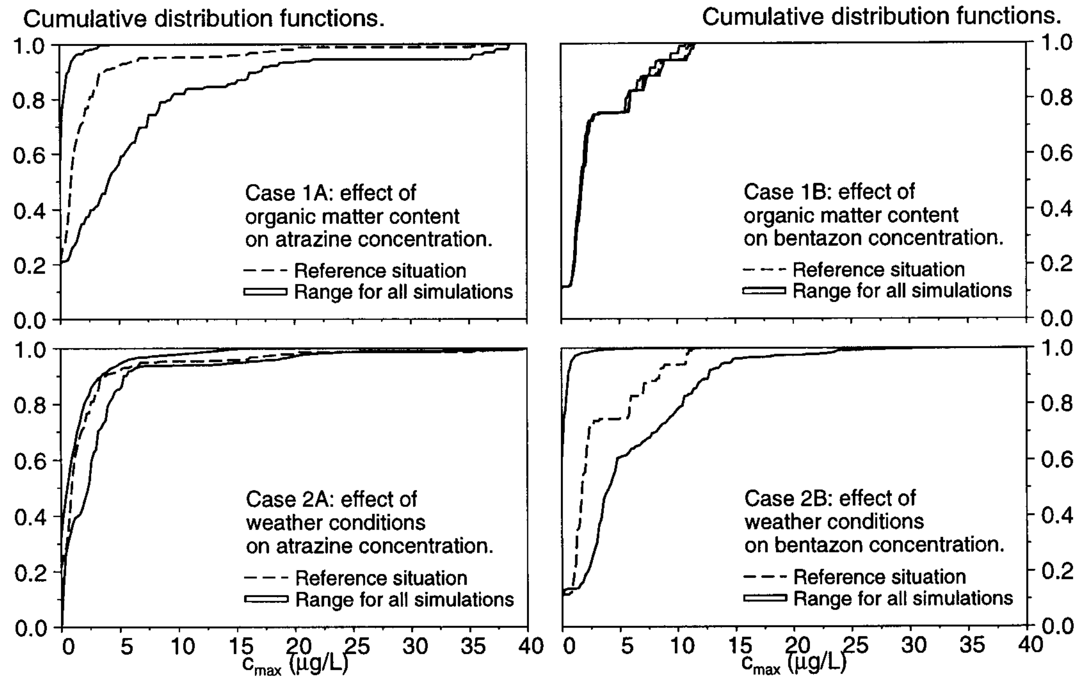


Figure 11

Cumulative distribution functions of the maps of the maximum concentration of atrazine (left) and bentazon (right), showing the effect of spatial variability of organic matter content and year-to-year variation of weather conditions.

5 LEACHING OF PESTICIDES IN 1993

The vulnerability maps shown in chapter 4 in combination with results from ISBEST were used to calculate maps of pesticide leaching. In section 5.1 some results from ISBEST are discussed. We used pesticide emission figures that were used for the evaluation of the Multi-year crop protection plan (Van der Linden *et al.*, 1996). These data refer to the year 1993. Results that are relevant to the leaching problem include the area on which the pesticides have been applied, and the average dose on those fields where these pesticides have actually been used. Section 5.2 discusses the actual pesticide leaching calculated with GEOPESTRAS. Relevant parameters are the maximum concentration of pesticide in the upper groundwater (an indicator of the quality of the environment), and the total amount of pesticide leached (a quantity indicator). In section 5.3 the total pesticide leaching to the groundwater is evaluated, and a summary map presented. Emphasis in the first two sections of this chapter is on the four pesticides dealt with in chapter 4. These pesticides not only have different chemical properties, they are also used in different crops and regions.

5.1 Geographical patterns of pesticide use

The geographical distribution of pesticide use has been estimated by investigating both the total use of a plant protection product over the country, and the spatial distribution of this use (see section 2.3). For the evaluation of the Multi-year crop protection plan, we used the data for the year 1993[2].

Results are shown in Figure 12 and Figure 13. Figure 12 shows the average dose (kg ha^{-1}) of atrazine, bentazone, chlorothalonile and dichloropropene at fields where those pesticides have actually been used, while Figure 13 shows the percentage of the area of agricultural land where those pesticides have actually been used. As expected, results in Figure 12 and Figure 13 are largely dependent upon the land-use map. Atrazine is a herbicide, and its use is confined to maize and asparagus. Thus, atrazine is primarily used on sandy soils in the Eastern and Southern part of the country. Bentazone is a herbicide as well, but it is used on a broader range of crops (grassland, maize, peas and beans). The map shows that it is used throughout the country. Chlorolothalonile is a fungicide, which is primarily used to protect against *Phytophthora* in potatoes, mildew in tomatoes, take-all disease in ornamental flowers, and various other fungi in onions and flower-bulbs. The nematicide dichloropropene is primarily used against eelworms. It is used in a variety of crops, the most important ones being potatoes, beets, onions, strawberries, and tree nurseries.

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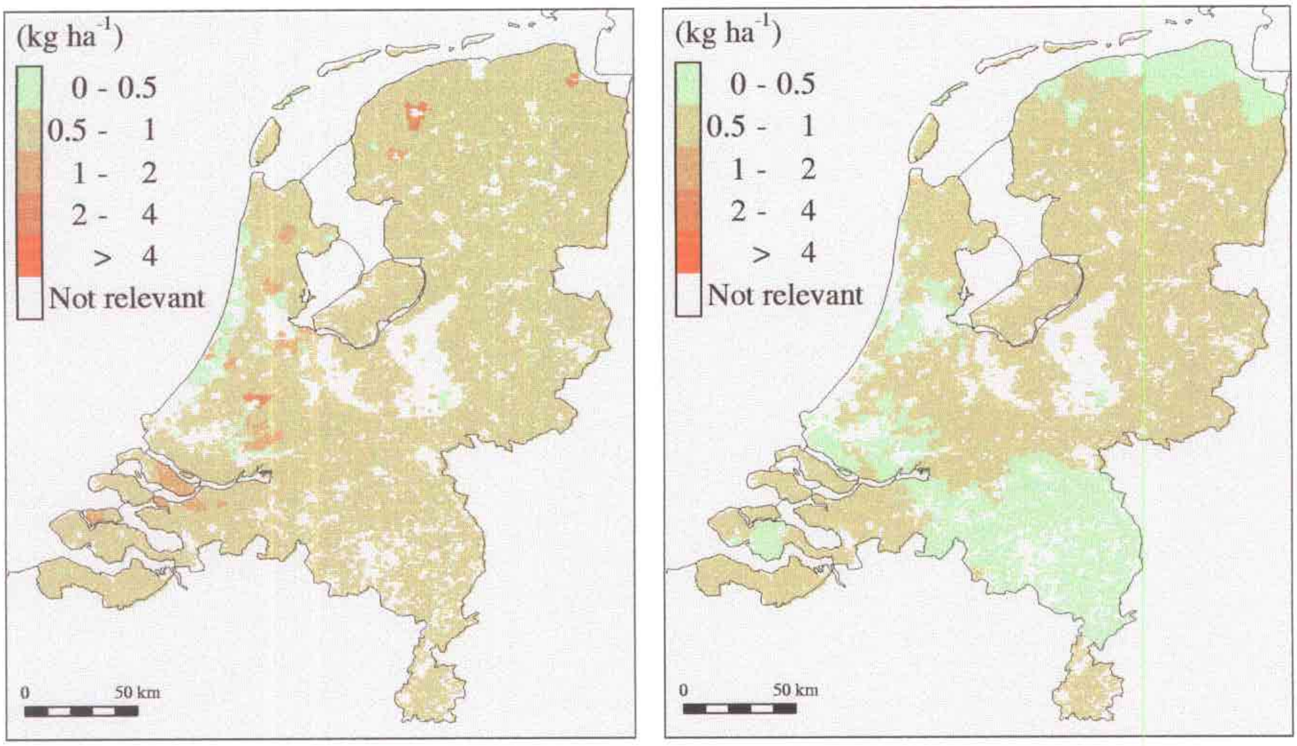
[2] In the final evaluation of the Multi-Year crop protection plan (Van der Linden, *et al.*, 1996), these data have been converted to data for the target year 1995 on the basis of the 1995 sales-figures.

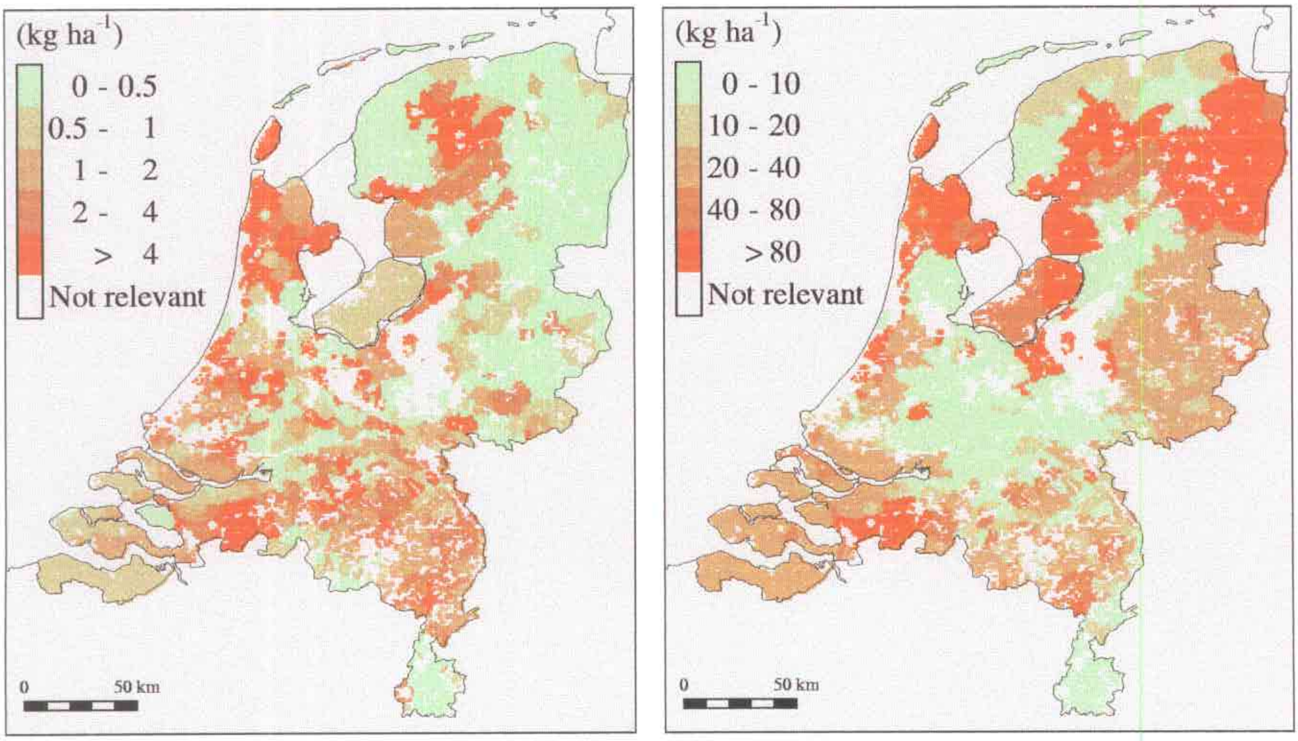
The two maps can best be interpreted in combination. As an example, atrazine is applied at moderate rates (usually 0.7 kg ha^{-1}), but over large areas. Dichloropropene is a representative of another extreme situation: It is used on rather small areas, but when it is used, a fairly large dose (often > 100 kg ha^{-1}) is given. Notice also that it may sometimes be confusing to read only one of the two maps. Figure 12, for example, suggests intensive usage of chlorothalonile in parts of the province of Friesland in the Northern part of the country, but Figure 13 shows that chlorothalonile is used on a small area in that part of the country. Further investigation learned that in this particular case high doses were given in tree nurseries (which occupy only a small part of the total area).

An interesting feature that can be seen from Figure 12 is that bentazone is used at a lower rate in the Southern part of the country than in the rest of the country. In this part of the country, where nitrogen inputs are rather high, herbicide stress is relatively high. For that reason, bentazone is used in combination with other herbicides for a more effective plant protection. A well known formulation is Laddok, which is a combination of atrazine and bentazone.

There is a reciprocal relationship between the area involved and the accuracy of the dosage estimated. This can best be explained with the maps of dichloropropene at hand. Dichloropropene is usually applied at a rate of 100-400 kg ha^{-1} (van der Plassche *et al.*, 1988). A lower dose than 100 kg ha^{-1} is not effective, so no farmer will give such a small dosage. Nonetheless, the map for dichloropropene suggests that in large parts of the country the application is at rates under 80 kg ha^{-1}, and the largest deviations occur in those areas where dichloropropene is used at small areas. This is due to the fact that the dosage as shown in Figure 12 is calculated by dividing the total pesticide use per municipality by the area where a pesticide has actually been used. As the accuracy of the estimated area decreases with it's magnitude, the estimated dosage also gets less accurate. It can be concluded that ISBEST gives a rather reliable geographical pattern of the pesticide dose for pesticides that are used over broad areas (atrazine and bentazone), but that the uncertainty in the predictions increases when the area at which a pesticide is used decreases (chlorothalonile and dichloropropene).


Atrazine (spring application)

Bentazone (spring application)

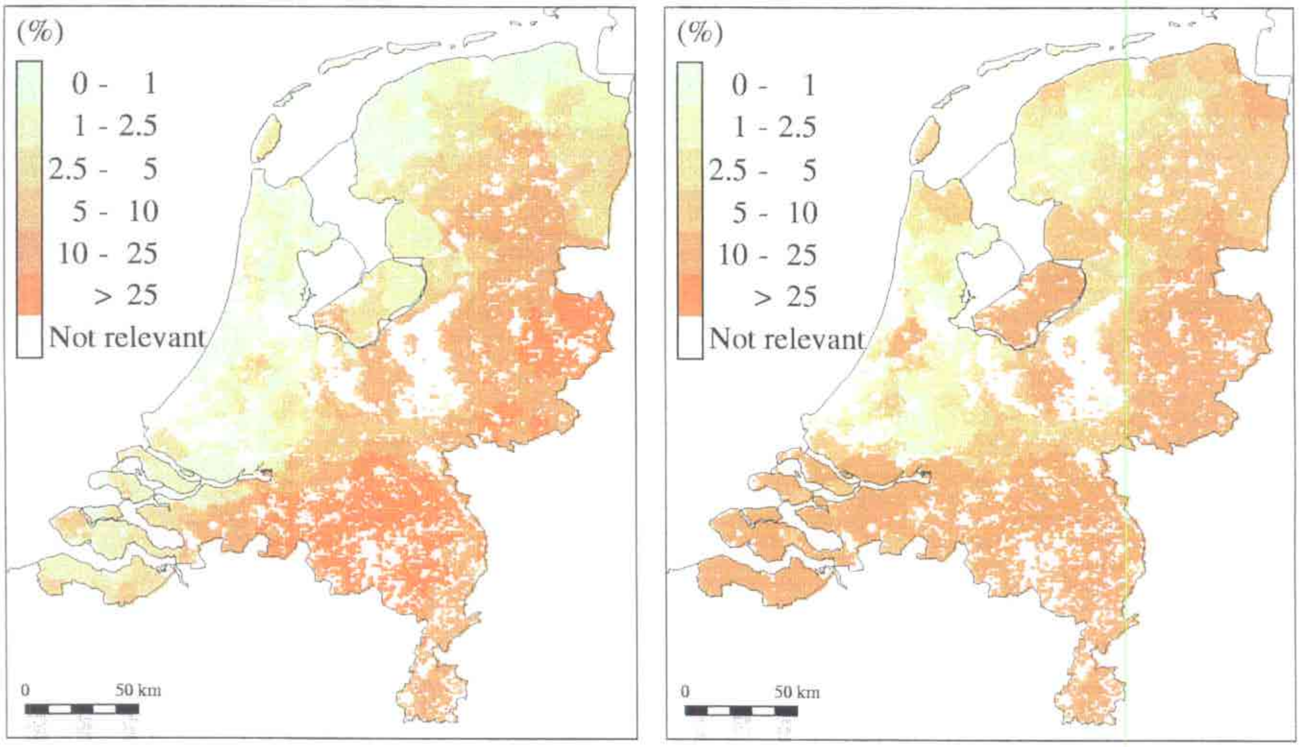

Hydroxy-chlorothalonile (spring applic.)

Dichloropropene (autumn application)

Figure 12

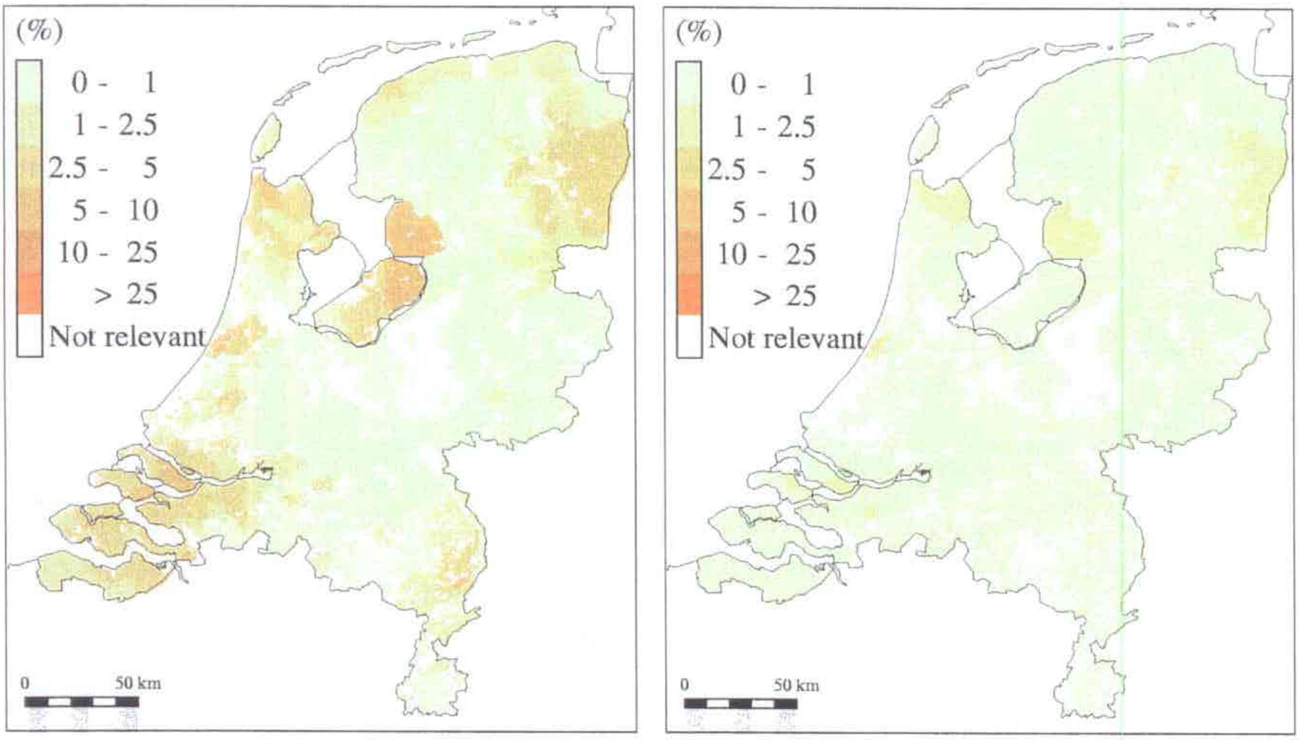
Average dose of four pesticides at fields where they have actually been used.

Notice that the classes for dichloropropene are different!



Atrazine (spring application)

Bentazone (spring application)



Hydroxy-chlorothalonile (spring applic.)

Dichloropropene (autumn application)

Figure 13
Percentage of the area of agricultural land where atrazine, bentazone, chlorothalonile and dichloropropene have actually been used.

5.2 Pesticide leaching on a regional scale

Actual leaching rates were obtained by multiplying the fraction leached (chapter 4) by the actual pesticide use. The actual maximum concentration of pesticide was obtained by multiplying the maximum concentration presented in chapter 4 by the average dose on treated fields (section 5.1). Moreover, the percentage of land where the maximum concentration exceeded the EU drinking-water standard (0.1 μg L^{-1}) was obtained by combining the concentrations with the area involved. Results of these calculations are presented in Figure 14-Figure 16 and table 10. For the explanation of these maps, both the information in chapter 4, and the information in section 5.1 must be considered.

Generally, concentrations of all pesticides are low in soils with a high organic matter content (peat soils in the Western and Northern part of the country). In these soils, organic matter contents are in such an order of magnitude that the resulting strong sorption of pesticides always counterbalances possible high pesticide use rates. In other words: These soils are not susceptible to pesticide leaching, even when a high pesticide dose is given.

Table 10 shows that approximately 75% of the area at which atrazine was applied is above the EU drinking-water standard of 0.1 μg L^{-1}. For bentazone, chlorothalonile and dichloropropene, these figures amounted to 90%, 75%, and 80%, respectively. The drinking-water standard was extremely exceeded (c_{max} > 10 μg L^{-1}) at significant areas for chlorothalonile and dichloropropene. Notice, however, that the total area where the drinking-water standard was exceeded amounted to almost 180000 ha for atrazine, whereas the drinking-water standard was exceeded at only 6235 ha for dichloropropene. In other words: *Two of the example pesticides (atrazine and bentazone) showed moderate concentrations over large areas, whereas the other two showed extreme concentrations over smaller areas.* We believe that it is highly relevant to consider both aspects of the pesticide leaching problem: From an (eco)toxicological point of view, extreme concentrations may be unacceptable. If, however, extreme concentration occur only at a small part of the area, the problem may remain manageable. One reason is that if the leaching occurs from only a small area, chemical dilution will occur in the saturated zone before a pesticide can reach drinking-water well.

Another way to present the pesticide leaching problem is to evaluate the total amount of pesticide leached (Figure 16), instead of the leachate concentration. The advantage of evaluating the amount (which is a 'quantity indicator') instead of the concentration in the soil-leachate (a 'quality indicator') is that problem areas can be identified with *one map* at hand. The major reason for this is that a map of the leaching rates inherently combines the information on the area involved, and the magnitude of the leaching. There is also a conceptually easy link to the pesticide use maps. However, there are also some disadvantages of evaluating amounts instead of the concentrations. Firstly, amounts do not really have an ecotoxicological meaning. Secondly, the EU drinking-water standard is based on concentrations. Nevertheless, Figure 16 shows the following general geographical patterns:

- for the four pesticides considered, the amount of pesticide leached is low in peat soils,
- considerable leaching of atrazine occurs from sandy soils,
- leaching of bentazone occurs throughout the country, with the exception of peat-soils,
- chlorothalonile leaching is primarily significant in the flower-bulb regions of the North-West, and in the South-Western part of the country (potatoes and onions).
- Dichloropropene leaching is high in the flower-bulb area of the North-West, and in the potato area of the 'Veenkoloniën' in the North-Eastern part of the country.

TABLE 10

Distribution of agricultural land over five concentration classes for four selected pesticides. The table summarizes both the area involved (ha), and the percentages of the total area at which each individual pesticide is applied.

c_{max}[a]	Atrazine[b]		Bentazone[b]		Chlorothalonile[b]		Dichloropropene[c]	
(µg L^{-1})	(%)	(ha)	(%)	(ha)	(%)	(ha)	(%)	(ha)
0-0.01	14.7	35025	0.4	80	18.0	5428	18.8	1481
0.01-0.1	10.6	25156	9.4	20246	6.2	1857	1.9	146
0.1-1	44.1	105030	39.0	83761	11.5	3461	0.6	45
1-10	30.0	71556	51.2	110120	34.0	10247	14.2	1117
> 10	0.6	1451	0.0	0	30.3	9123	64.5	5073
Total	100.0	238218	100.0	214927	100.0	30116	100.0	7862

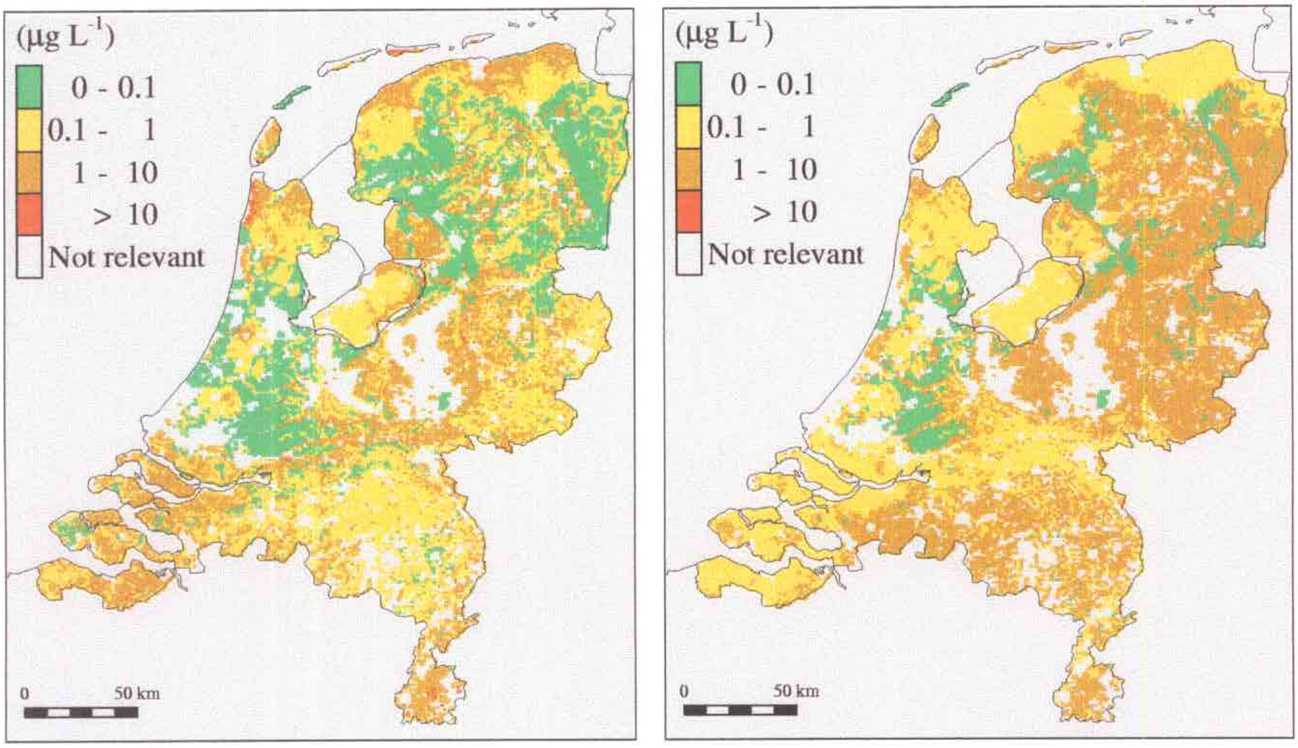
[a] refers to the maximum concentration in time

[b] spring application

[c] autumn application

Atrazine (spring application)

Bentazone (spring application)



Chlorothalonile (spring application)

Dichloropropene (autumn application)

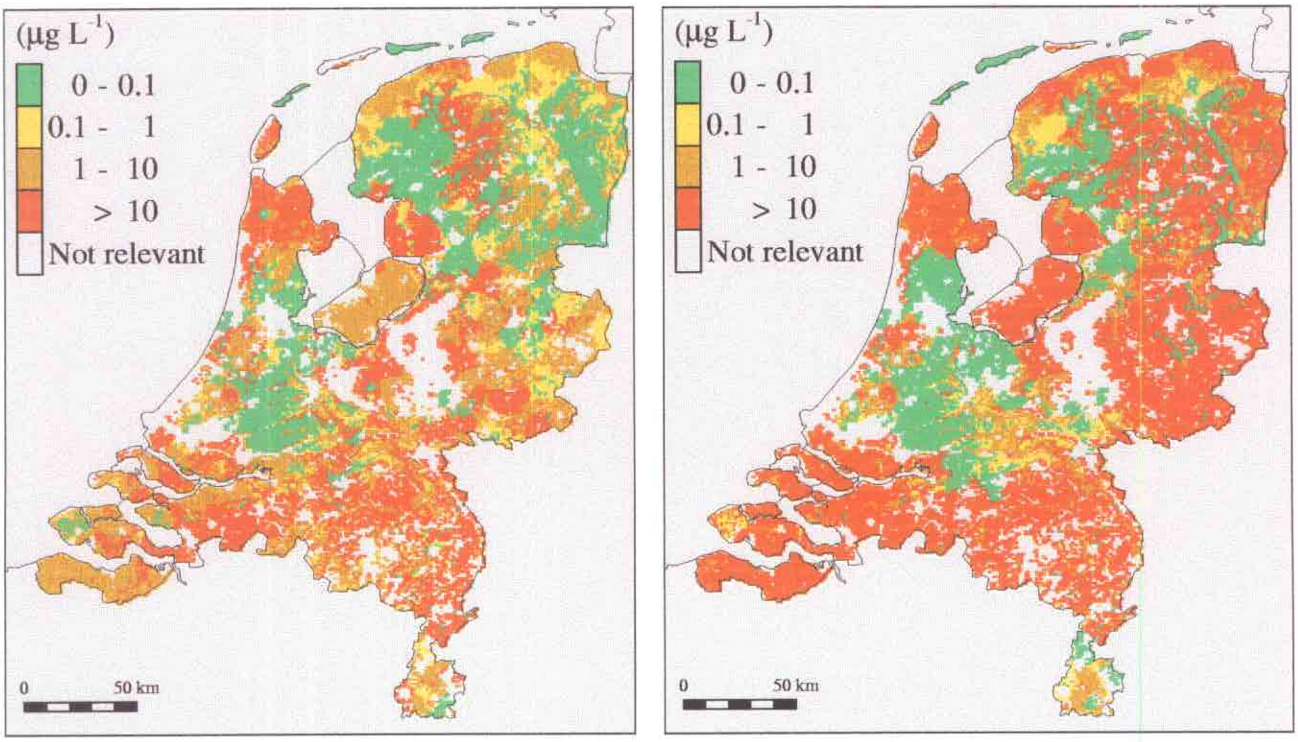
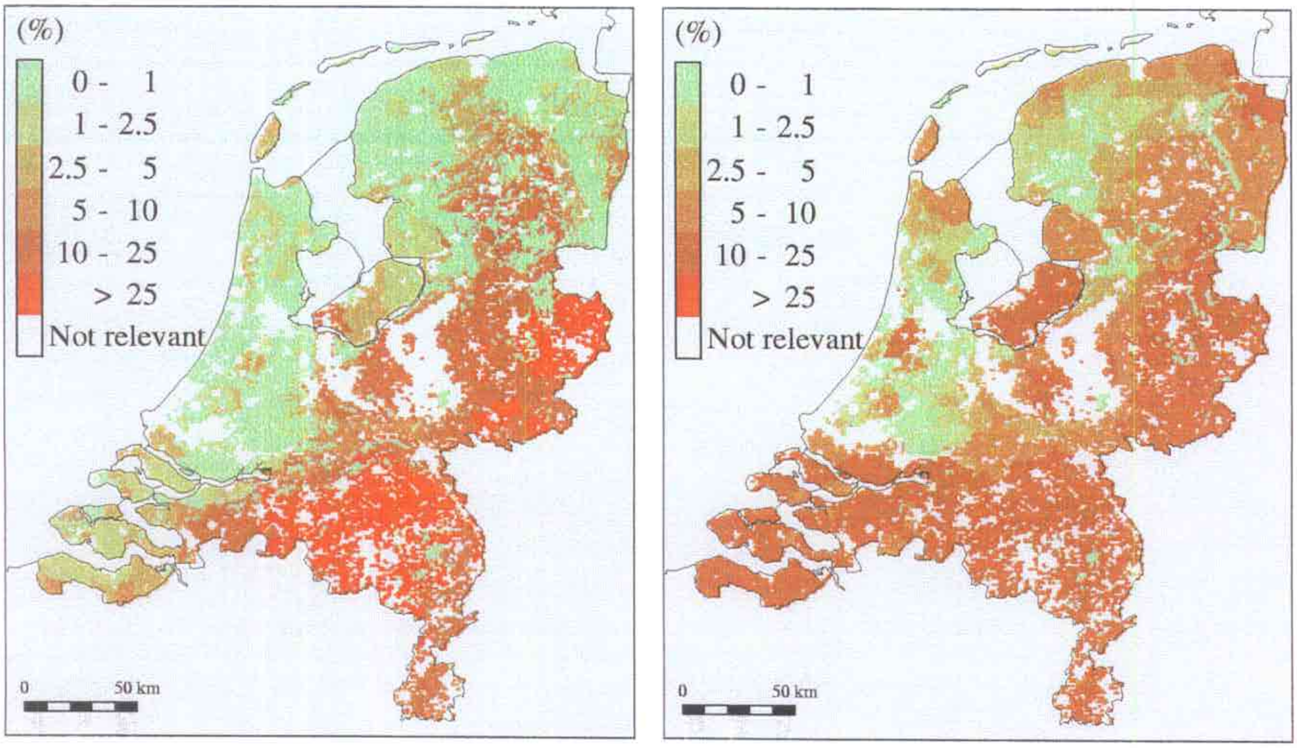


Figure 14

Average maximun concentration of pesticide in the 1-2 m soil layer, using the actual dose. Averages are valid for the area where the pesticides have actually been used. Please be beware of the fact that this area may be rather small, as shown in the maps on the facing page.

Atrazine (spring application)

Bentazone (spring application)



Chlorothalonile (spring application)

Dichloropropene (autumn application)

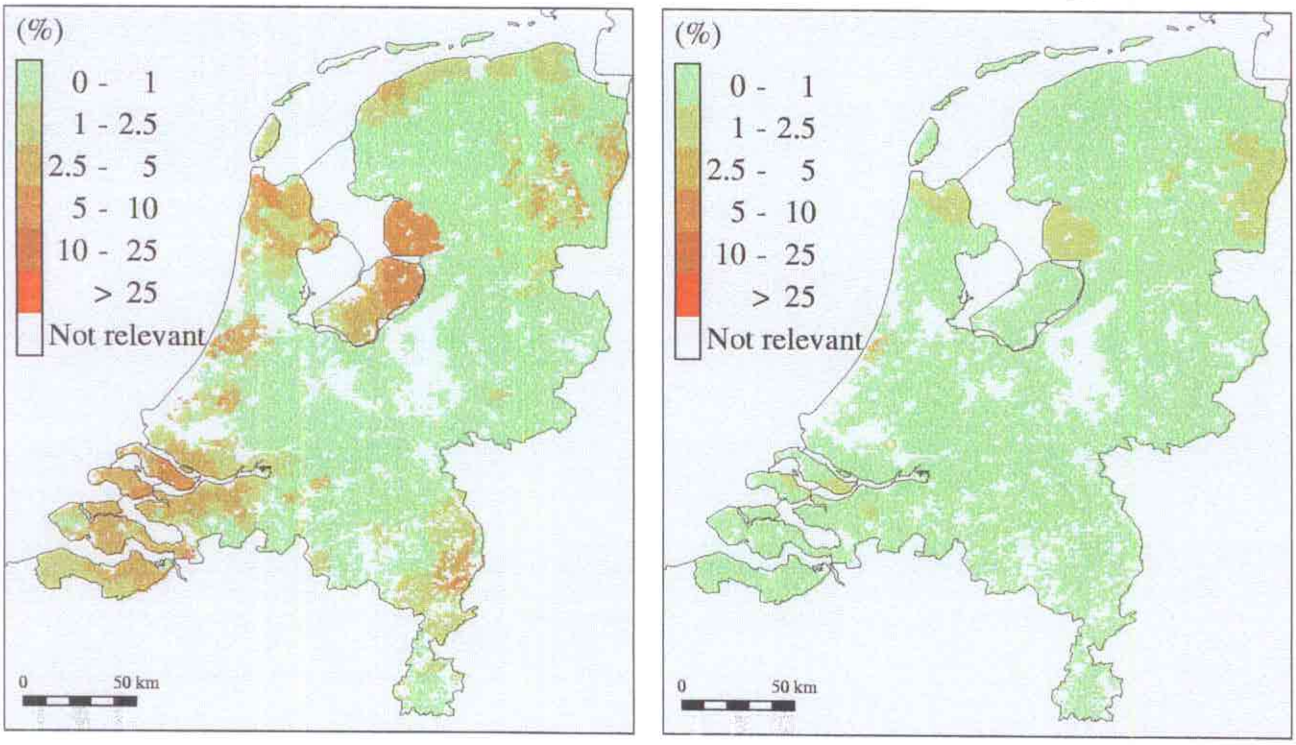
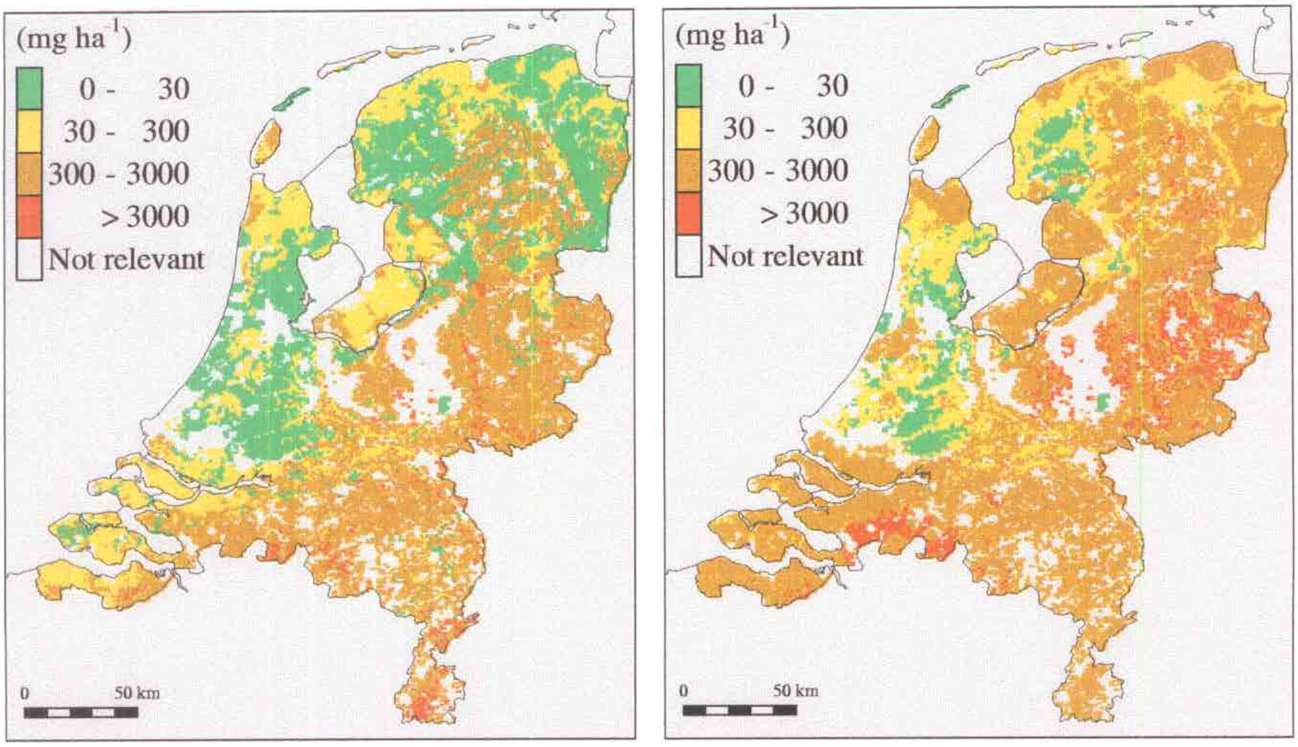


Figure 15

Percentage of the area of agricultural land with a concentration of pesticide above the EU-drinking water standard of 0.1 $\mu g\ L^{-1}$*. Notice that the exceedance can be high or low, as shown by the maps on the facing page.*

Atrazine

Bentazone



Chlorothalonile

Dichloropropene.

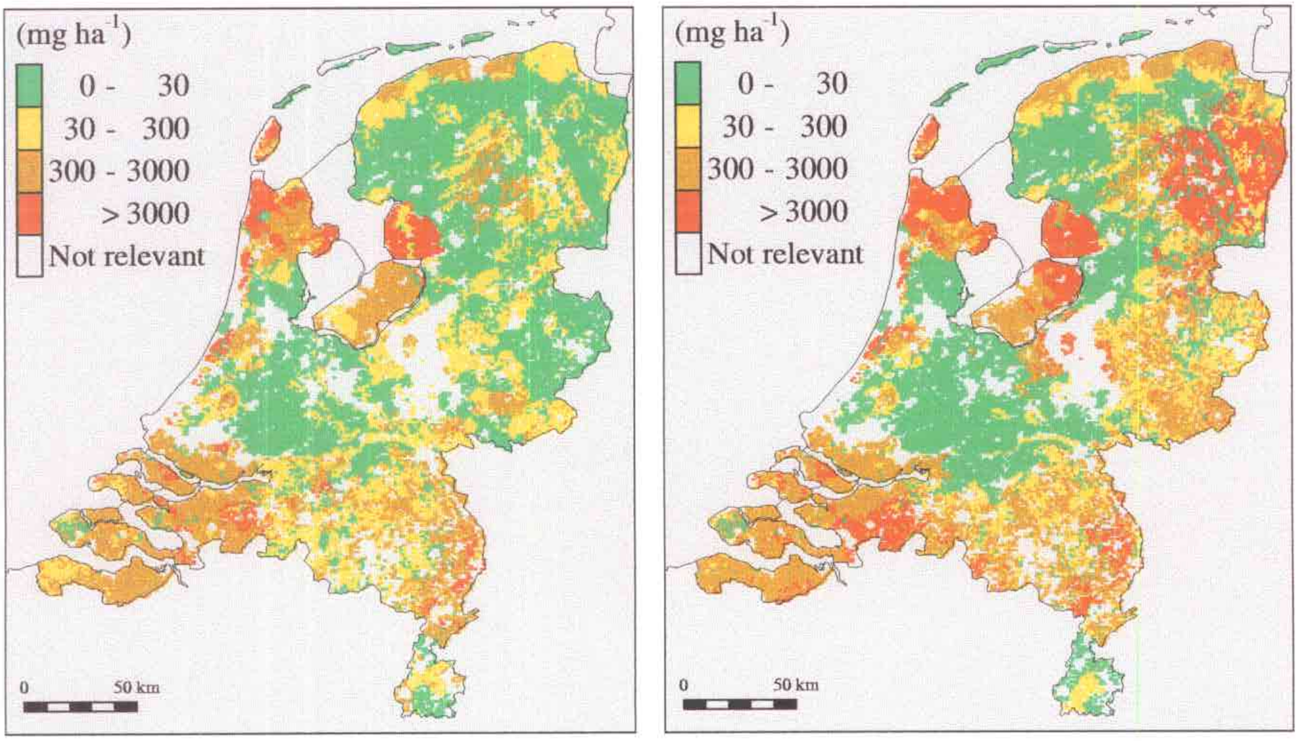


Figure 16

Grid-cell average leaching rate (mg ha^{-1}) of four selected pesticides to the shallow groundwater. Spring and autumn applications have been summed. The maps refer to the year 1993. A leaching rate of 30 mg ha^{-1} is approximately equivalent with a concentration of 0.1 µg L^{-1}.

5.3 Evaluation of the total pesticide emission to the groundwater

Within the framework of the evaluation of the Multi-Year crop protection plan (Van der Linden *et al.*, 1996), GEOPESTRAS was used to calculate the total emission of all pesticides to the upper groundwater. As the total number of admitted pesticides in the Netherlands is approximately 350, it was not feasible to carry out GEOPESTRAS runs for all these pesticides. Instead, a mixed approach was followed (see also Figure 17):

- Firstly, we checked whether data on the behaviour of a pesticide in soil were available. If these data were not available, we estimated the total leaching rate for that particular pesticide by multiplying its total use with a leaching fraction. This leaching fraction was set equal to the median leaching fraction for all admitted pesticides. It's estimated value was 0.001% of the applied dose. It must be noticed that data on the behaviour in soil were only unavailable for pesticides that were used in small quantities.
- If data on the behaviour of a pesticide in soil were available, a more realistic leaching fraction could be substituted. This leaching fraction was derived by running the model PESTLA (Boesten and Van der Linden, 1991) with a standard dataset (i.e. one surface application of pesticide in an initially pesticide free humic sandy soil, continuous cropping with maize, groundwater table at a fixed depth of 1 m, and weather data for the year 1980). For a total number of 200 combinations of DT_{50} and K_{om}, the leaching fraction was calculated for the standard dataset. It turned out that only 17 pesticides showed a leaching in excess of 100 kg.
- Finally, pesticides that were expected to leach in excess of 100 kg were subjected to a detailed evaluation with GEOPESTRAS as described in this report.

Results of the detailed calculations are presented in table 11. The calculated total leaching of the 17 selected pesticides to the shallow groundwater was somewhat more than 43000 kg. The total leaching of all other pesticides was estimated at 8000 kg (Van der Linden *et al.*, 1996), so the selected pesticides covered almost 80% of the total leaching. Additional calculations with a model to calculate loads on surface water (PESCO; Kraaij *et al.*, 1994) showed that approximately 53% of the total load (27000 kg) leached to the deep groundwater, while the remainder (24000 kg) instantaneously reached the surface water through artificial drains.

In Figure 18 a summary map is presented. This map was created by summing on a gridcell basis the leaching rate for the selected pesticides. The highest pesticide leaching rates occurred in the following areas:

- The 'Veenkoloniën' in the North-Eastern part of the country. In this region, the nematicides dichloropropene and metam-sodium were most commonly used.
- The flower bulb areas in the North-Western part of the country. In these areas, both nematicides (aldicarb, metam-sodium and dichloropropene), and fungicides (e.g. chlorothalonile) were used.

- The sandy soils of the province of Brabant in the Southern part of the country. Here bentazone is widely used.

Figure 18 also shows that in the Eastern part of the country the total leaching of pesticides is significantly lower than in the province of Brabant. This is primarily due to the fact that in Noord-Brabant the herbicide bentazone is commonly used, whereas in the Eastern parts of the country atrazine is more often used. Bentazone has a larger leaching potential than atrazine.

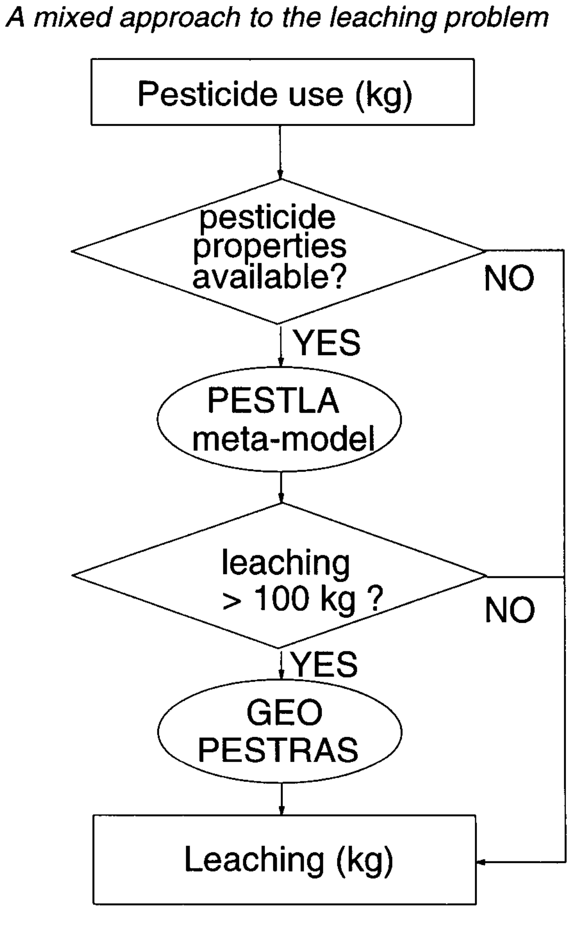


Figure 17
Diagram of the selection method for the various pesticides.

TABLE 11

Calculated leaching of 17 mobile pesticides[a] to the shallow groundwater in 1993, and the area where the pesticides have been used.

Pesticide	Time of application	Fraction of dose	Leaching from the upper meter[c]		Area at which the pesticide was used	
		%[b]	kg	class[d]	km^2	%[e]
aldicarb	spring	83	176	A	321	1.6
	autumn	17	836	F	66	0.3
atrazine	spring	100	1871	C	2300	11.7
bentazone	spring	93	1373	C	1987	9.3
	autumn	7	820	F	139	0.7
carbofuran	spring	99	210	C	63	0.3
	autumn	1	4	E	1	0.0
chlorothalonile	spring	100	841	D	295	1.5
carbendazim[f]	spring	99	152	B	481	2.5
	autumn	1	2	C	5	0.0
chloridazon	spring	100	100	B	612	3.3
cis-1,3-DCP	spring	5	23	A	4	0.0
	autumn	95	7634	C	69	0.3
dicamba	spring	100	326	F	259	1.4
lenacil	spring	100	1841	F	53	0.3
mecoprop-p	spring	30	146	B	527	2.6
	autumn	70	7312	E	1229	6.2
metalaxyl	spring	94	235	E	104	0.5
	autumn	6	22	E	7	0.0
metam-sodium	spring	5	17	A	54	0.3
	autumn	95	15469	C	989	5.2
metolachlor	spring	100	476	B	192	1.0
oxamyl	spring	65	76	F	38	0.2
	autumn	35	452	F	21	0.1
pendimethalin	spring	100	386	D	97	0.5
pyridate	spring	100	2385	D	838	4.3
Total of selected pesticides (rounded)			43000			
Other pesticides (see text)			8000			
TOTAL			**51000**			
To deep groundwater			27000			
To surface water			24000			

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[a] Data are available for a total number of 350 pesticides. However, simulations with GEOPESTRAS were only carried out for those pesticides that were expected to leach in excess of 100 kg.

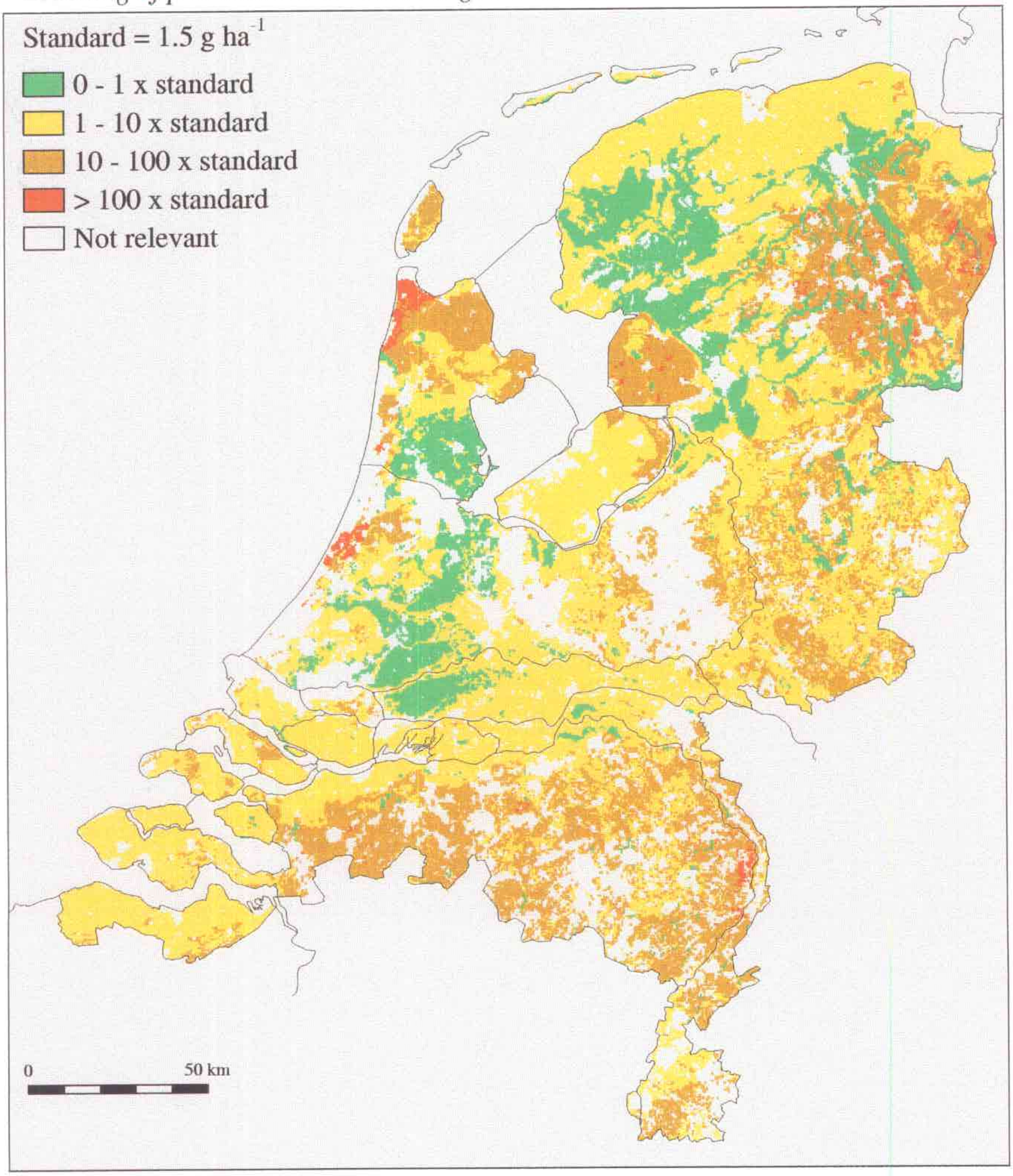
[b] Percentage of the total annual dose applied in spring and autumn, respectively.

[c] Leaching from the upper meter of the soil profile, regardless of the groundwater level.

[d] Class A: leaching < 0.1 % of the total dose, class B: 0.1-1%, class C: 1-2.5%, class D: 2.5-5%, class E: 5-10%, class F: > 10%.

[e] Percentage of the total area.

[f] After subtraction of 43% of the total dose for use in immersion bathes.



Leaching of pesticides to the shallow groundwater.

Figure 18

Grid-cell average total leaching rate of 17 pesticides to the shallow groundwater. Spring and autumn applications were summed. The maps refer to the year 1993. The drinking-water standard of 0.5 µg L^{-1} was converted to a rate of 1.50 g ha^{-1} on the basis of an annual precipitation surplus of 300 mm a^{-1}.

6 CONCLUSIONS

The regional-scale pesticide leaching model GEOPESTRAS in combination with the information system on pesticide use ISBEST proved to be a powerful and flexible tool in assessing both the magnitude of the leaching, and the area involved. Results were also suitable for evaluating spatial scenario's. Using the mega-plot approach described in this report, the number of point locations for which the model had to be run to get spatial patterns for The Netherlands could be effectively reduced from 93000 to a manageable 897. The method of regionalization described in this report is flexible, so it can easily be adapted for other spatial scales (for example when variation in temperature must be taken into account). Moreover, as the underlying model is a process-oriented model, a broad range of pesticides could be considered.

Results showed that the calculated spatial pattern of pesticide leaching strongly depended upon the pesticide properties. The calculated concentration of pesticide in the soil leachate was most dependent upon the organic matter content in the case of moderately mobile and moderately degradable pesticides (e.g. atrazine). On the other hand, concentrations of mobile pesticides (bentazone and chlorothalonile) were strongly correlated to the soil physical properties, and concentrations of volatile pesticides depended strongly upon both the ground-water level, and the soil physical properties. This demonstrates that general conclusions on the underlying processes could not be drawn from results for a single pesticide, or a single parameter (e.g. organic matter content).

The total calculated leaching in 1993 was 51000 kg. Additional calculations showed that approximately 53% of the total load leached to the deep groundwater, while the remainder (24000 kg) instantaneously reached the surface water through artificial drains. Peat soils were generally invulnerable to pesticide leaching, whereas sandy and loamy soils with low organic matter contents were very vulnerable (concentration often above 1 $\mu g\ L^{-1}$). The highest pesticide leaching occurred in the 'Veenkoloniën' to the North-East, the flower-bulb area of the North-West, and the sandy soils of the province of Noord-Brabant to the South. Approximately 75% of the area at which atrazine was applied was above the EU drinking-water standard of 0.1 $\mu g\ L^{-1}$. For bentazone, hydroxy-chlorothalonile and dichloropropene, these figures amounted to 90%, 75%, and 80%, respectively. Bentazone and atrazine were used over large areas, but did not show extreme concentrations. Chlorothalonile and dichloropropene, on the other hand, showed extreme concentrations (> 10 $\mu g\ L^{-1}$), but were used at smaller areas. This example showed that the combined information of the area, and the magnitude of the leaching was highly significant.

The model results can be used to classify the leaching from soils on a relative scale, and can be used to answer such questions as 'In what regions can a certain pesticide be expected to leach in excess of established environmental standards?'. It is nevertheless interesting to verify the absolute range of the predictions. Past field tests of the underlying model have primarily been carried out in sandy soils. This implies that the uncertainty of the model results is higher in finer-textured soils than in sandy soils. Field tests under a broader range of conditions (viz. finer-textured soils) are therefore a clear research need for the near future. Such field tests should include an evaluation of the effects of the hypothesized relationships and assumptions in the model (no preferential flow; equilibrium sorption; depth-dependence of degradation; surface-volatilization, etc.), and quality of model input data.

GEOPESTRAS may provide the input for other dispersion models, such as:
- a model to calculate loads on surface water (PESCO),
- a model to calculate the dispersion of pesticides in aquifers (LGMCAD),
- a model to calculate the dispersion of volatile pesticides in the atmosphere.

Actions must be undertaken to improvide the coupling between GEOPESTRAS and these models, especially when feed-back mechanisms cannot be ignored. Another concern for the near future is the spatial resolution of the Information System on Pesticide Use. A last point to be mentioned is the increasing efficiency of pesticides, so that they can be applied at lower dosages. From an ecotoxicological point of view, the EU drinking-water standard may no longer be sufficient. We therefore strongly recommend the incorporation of standards based on ecotoxicological research in this kind of analyses.

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