Cost-effective risk assessment of pesticide leaching at field scales: quality versus quantity of information

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ABSTRACT

This paper addresses the issue of how to obtain effectively and efficiently the information needed as the input parameters for pesticide leaching models, in the context of risk assessment at the field scale. A key question is the extent to which low-cost/less-accurate information at a number of locations in the field is more useful than high-cost/more-accurate information on a few (even single) samples. An example is presented which considers the balance between quality and quantity of information for several soil properties, including soil texture, soil organic matter, adsorption and degradation, based on the spatial variation in the predicted leaching losses of isoproturon from a sandy loam soil in southern England.

INTRODUCTION

It is not feasible to assess pesticide leaching at the field scale by integrating direct measurements of leaching from all parts of the field. Instead, conclusions are reached by studying sub-samples taken from the field, either by direct experiment (e.g. using lysimeters) or by modelling. Simulation models have become indispensable research tools for describing movement of water and solutes into and through the unsaturated zone (Wösten *et al.*, 1990) and are increasingly used in pesticide registration procedures.

Geostatistics optimises the interpolation between sampling sites, providing a powerful tool for predicting values of a soil property at points where no observations have been made, or over larger areas of land (Oliver *et al.*, 1996). As a result, fewer sampling sites are needed to achieve the same level of precision (Di *et al.*, 1989). An obvious next step is the application of geostatistical techniques to field measurements, generating inputs to solute transport models, and carrying out distributed modelling to predict spatial patterns of leaching within the field.

Oliver *et al.*, (1999) used the LEACHP model, in combination with geostatistics, to predict leaching of atrazine at the field scale. The simulation results predicted that significant losses of atrazine below 1 m depth would have occurred from just 10% of the field and that the contribution from the rest of the field was negligible. They concluded that, when pesticide leaching is marginal, most of the pesticide leached at the field scale is likely to be contributed by vulnerable zones that comprise a relatively small proportion of the total land area.

The identification of vulnerable zones within fields requires spatially distributed sampling involving large numbers of samples, and this has severe logistical implications. For example, pesticide transport models require parameterisation of adsorption, degradation and soil hydrodynamic properties. Since soil hydrodynamic properties are difficult to measure in the field, pedotransfer functions (PTFs) have been developed to estimate the properties from measurements of soil organic matter (SOM), bulk density (BD) and particle size distribution (PSD) (Brooks & Corey, 1964; Mualem, 1976; Van Genuchten, 1980; Hutson & Cass, 1987; Tietje & Tapkenhinrichs, 1993).

Such an approach simplifies the measurements to be made but does not decrease the amount of data required. For example, prediction of soil hydrodynamic properties in a single field using PTFs can require three measurements (PSD, SOM, BD) at three depths at each point. Geostatistics requires at least 100 data points (Oliver *et al.*, 1996) giving a total of 900 laboratory determinations.

Therefore the laboratory measurements need to be reduced to minimise the total workload, but not at the expense of predictive accuracy. It can be argued that, where the variability of soil properties is high or a high level of precision in interpolation is desired, the number of sampling sites cannot be substantially reduced (Scheinost & Schwertmann, 1995). However, although spatial variation of a given parameter may be great, solute transport models may not be sensitive to that variation and it may be possible to reduce the number of measurements or use a single, average value for the field. When the parameter varies spatially, and the model is sensitive to that variation, the combined use of surrogate measurements at many locations and empirical relationships to transform the data may prove a better alternative. Therefore design of cost-efficient sampling strategies for risk assessment of pesticide leaching at the field scale must include consideration of model sensitivity to parameter variation.

Oliver *et al.*,(1999) concluded that spatial variation in SOM content (associated with pesticide sorption and degradation) was very much more important in influencing the leaching of atrazine than was spatial variability in the soil hydrodynamic properties controlling the downward movement of pesticides via matrix flow. Similar results were reported by Soutter & Musy (1999). Therefore, it may be feasible to reduce the number of points where soil hydrodynamic properties are estimated and still be able to identify those zones within a field that are vulnerable to leaching.

Dubus *et al.*,(2000) tested four pesticide leaching models for sensitivity to input parameters and concluded that the most important criteria are: the adsorption parameters (Freundlich coefficient and exponent); pesticide half-life; SOM content and bulk density. This paper investigates the effect of spatial variation in these properties on the spatial variation in the predicted leaching losses of isoproturon from a sandy loam soil in southern England.

MATERIALS AND METHODS

The study site was a 9 ha arable field situated on a river terrace adjacent to the River Thames near Reading. The soil is Sonning Series, a freely-draining light sandy loam overlying alluvial gravel. The field was surveyed in 1998 and a total of 90 samples were collected from the top 0-15 cm using a 5-stage unbalanced nested sampling scheme as described by Oliver & Webster (1986). Pesticide leaching losses from the top 30 cm were predicted using the pesticide leaching model SWAP (version 2.0.7d, January 2000). The input data were either measured (PSD, DT_{50}, Kd) or calculated using PTFs (SOM, BD).

Particle size distribution was determined on the 2 mm fraction by laser granulometry. Pesticide degradation rate (DT_{50}) was estimated by incubation with isoproturon (IPU) for 7 and 28 days. Duplicate samples of fresh soil (equivalent to 30 g oven dry soil) were weighed into glass jars. A suspension of commercial formulation of IPU (Alpha isoproturon 500, 46.4% a.i.) in water was added to produce a dose concentration of 13.2 mg/kg. The soil was incubated at 20°C and the moisture content was maintained at 50% maximum water holding capacity. The samples were extracted with 90 ml acetonitrile:water (70:30 mix), a small aliquot was passed through a 0.2 μm membrane filter and analysed by hplc (Zorbex ODS; 5 μm column; flowrate 0.8 ml/min; detection by u.v. at 240 nm).

Loss on ignition (LOI) was determined by ignition of oven dried soil at 450°C for 24 h. SOM was estimated from LOI using a field-specific PTF following the procedure described by Frogbrook & Oliver (2001). Geostatistical techniques were used to produce a map of LOI. Nine samples (three each from the high, medium and low LOI areas) were identified for determination of soil organic carbon (SOC) using the modified Walkley-Black procedure (MAFF, 1986). The nine LOI and SOC determinations were used to produce a PTF for SOM.

Kd was determined for all samples by equilibrium with 0.02M $CaCl_2$ containing 5 mg/l IPU (5 g soil:20 ml solution), assuming linear adsorption. The Freundlich exponent was kept constant at 1.0 because adsorption experiments on four samples showed that adsorption was linear in the range of concentrations modelled. Bulk density was calculated using a PTF for ploughed topsoils (Chen, 1998):

$$BD = 1.483 - 0.447C + 0.141S - 3.97SOM$$

where C = mass fraction of clay
S = mass fraction of sand
SOM = mass fraction of soil organic matter

Water release characteristics were calculated using a PTF within the model using the analytical function option (Mualem-van Genuchten equation) and PSD, SOM and BD.

Weather data (12 months) were selected from long-term measurements at the Reading University weather station (Sonning, Berkshire, UK). Potential evapotranspiration was calculated outside the model using the Penman-Monteith formula. The weather data were repeated to give a simulation run of three years, providing 2 years to allow the soil water status to stabilise. A crop (SWAP standard maize data) was used (sown 1 May, harvest 15 October each year). Pesticide was applied at the rate of 2.5 kg a.i./ha on 15 March of the third simulation year.

RESULTS AND DISCUSSION

The model was run six times for each of the 90 field locations. The first run was the base scenario where all spatially variable input parameters (Table 1) were as measured or calculated. For each of the subsequent runs one of the parameters was held constant at the field average value.

The model accounted for between 99.92 and 100% of the pesticide applied (Table 2). At the end of the three year simulation all the pesticide had gone from the top 30 cm of the profile, except for three of the 90 locations which had slow degradation rates (DT_{50} more than 30 days).

Table 1. Spatial variability in the input data for the pesticide leaching model, SWAP

	%Clay	%Silt	%Sand	SOM%	Kd ml/g	DT_{50} days	BD g/cm^3
Maximum	15.04	30.93	70.91	4.092	2.14	37.37	1.4819
Minimum	6.45	21.05	54.03	1.677	0.48	8.70	1.3828
Mean	8.46	25.74	65.81	2.728	1.25	20.54	1.4297
Median	7.69	25.50	66.78	2.767	1.26	20.75	1.4283
Std Dev	1.92	2.16	3.97	0.492	0.35	4.85	0.0278
Skew	1.22	0.13	-0.76	0.322	0.35	0.65	-0.1721

Table 2. Spatial variability in leaching of IPU (g/ha) at 30 cm predicted using SWAP for six scenarios, with all parameters varying (base scenario) or substitution of the mean value for one parameter

	Base Scenario	Mean PSD	Mean Bulk Density	Mean Organic Matter	Mean Kd	Mean DT_{50}
Maximum	318	317	315	317	312	261
Minimum	0	0	0	0	0	0
Mean	47	46	46	46	43	43
Std Dev	49	48	48	48	52	37
CV%	104.2	104.2	103.9	104.2	121.1	87.6
Skew	2.46	2.48	2.50	2.47	3.39	2.47
RMSE		1.64	2.37	1.23	53.7	46.9

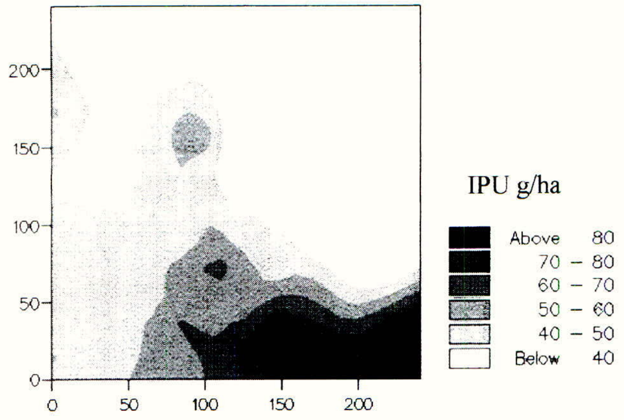

Figure 1. Predicted spatial variation in leaching at 30 cm (base scenario)

In the base scenario the average amount leached at 30 cm was 47 g/ha, representing 1.9% of pesticide applied. Analysis of the variation in leaching between the locations shows that 50% of leaching was accounted for by 72 out of 90 locations and 50% by 18 locations. This confirms the bias in leaching toward a small number of locations within the field (Figure 1).

Substituting the field mean value for PSD, BD or SOM had little effect on the mean or range of amount leached. All three scenarios accounted for between 98.3% and 99.4% of the aggregated leaching of the 90 locations. The mean DT_{50} and Kd scenarios accounted for 91.7% and 92.8% of the aggregated leaching respectively. This indicates that the total predicted leaching from the field could probably be estimated from field average values of these parameters, on condition that the measured value is a true estimate of the field mean. The number of samples (n) required to estimate the field mean depends on the within-field variation (standard deviation, σ), the model sensitivity to parameter (tolerance required, L) and the confidence level required for the result (Student's-t, Z):

$$n = (Z * \sigma)^2/L^2$$

The model is very sensitive to variation in DT_{50} and Kd, and these parameters also had the greatest within-field variation. Therefore, for accurate estimation of the average field leaching, it would be more effective to take many (23) measurements of DT_{50} and Kd within the field compared with few (2) measurements of particle size distribution.

Prediction of leaching vulnerable zones within the field shows similar sensitivity to DT_{50}. There was no significant difference ($R > 0.98$) between the first four scenarios in Table 2 as indicated by the small differences in range, mean, standard deviation and skew. By using the mean DT_{50} much of the variation in predicted leaching was removed, resulting in a narrower range of values.

The root mean square error (RMSE) was calculated (Table 2) to compare the accuracy of each of the predictions compared with the base scenario. Comparison of RMSE shows that the accuracy depends on Kd > DT_{50} >> BD > PSD > SOM and that the RMSE for DT_{50} and Kd is an order of magnitude greater than for the other parameters. These results differ somewhat from those reported by Dubus *et al.* (2000), who predicted that the relative importance of the parameters decreased in the order Kd > DT_{50} > SOM > BD > PSD for a similar compound and soil type.

CONCLUSIONS

These results indicate that spatial variation in pesticide half-life and adsorption are the most important parameters for the estimation of total pesticide leaching and spatial variation in leaching. But the results should be treated with caution: firstly, they are the results from only one model that utilises a simplified pesticide fate routine. They refer to results for only one pesticide and one field. Two parameters have been ignored that were identified as significant by Dubus *et al.*, (2000), namely the Freundlich exponent and preferential flow. Work is currently in progress to investigate how these vary at the field scale.

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Metamodeling to assess pesticides leaching on a wide scale

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ABSTRACT

A simplified meta-model methodology has been applied to assess the spatial distribution of potential groundwater contamination from pesticides. The approach is based on a one-dimensional leaching model (LEACHP) linked to a geographic information system (GIS). A statistical technique to summarise the model input-output relationships (stepwise regression procedure) in order to upscale the estimated concentrations. The potential for atrazine leaching was estimated for the agricultural area of Piacenza province (Northern Italy).

INTRODUCTION

In the last decades an increasing number of mathematical models to predict environmental fate of pesticides have been developed, with particular attention to pesticides leaching. However, because of the amount of input data and the large numbers of simulations required to cover large areas (regional/national), these physically based techniques are generally time-consuming and economically unfavourable. Thus, it is required a methodology to extrapolate results from local scale to a nation-wide scale taking into account at the same time the geographic variability of the model input parameters.

We developed an approach based on a one-dimensional leaching model (LEACHP) linked to a geographic information system (GIS) and a statistical technique to summarise the model input-output relationships (stepwise regression procedure) in order to upscale the estimated concentrations. The resulting frequency distributions map of the pesticide leaching concentrations can be used in sustainable groundwater management and decision making.

MATERIALS AND METHODS

Pesticide Leaching Model

The pesticide fate and transport model LEACHP (Wagenet & Hutson, 1995) was used for this study. LEACHP is a one-dimensional finite difference model describing the water and chemical regime in unsatured or partially saturated soil profiles. All spatially-distributed parameters required as input by the model (soil type, crop type, climate and hydrology) were stored in a GIS database. Figure 1 shows the linkage between the database and the model. In this *loose coupling* (Corwin *et al.*, 1997), the GIS (ESRI ArcView, 1996) is used to create external text files consisting of input data for the model. Afterwards the output files resulting from simulations are read and processed to create leaching pesticide concentration maps.

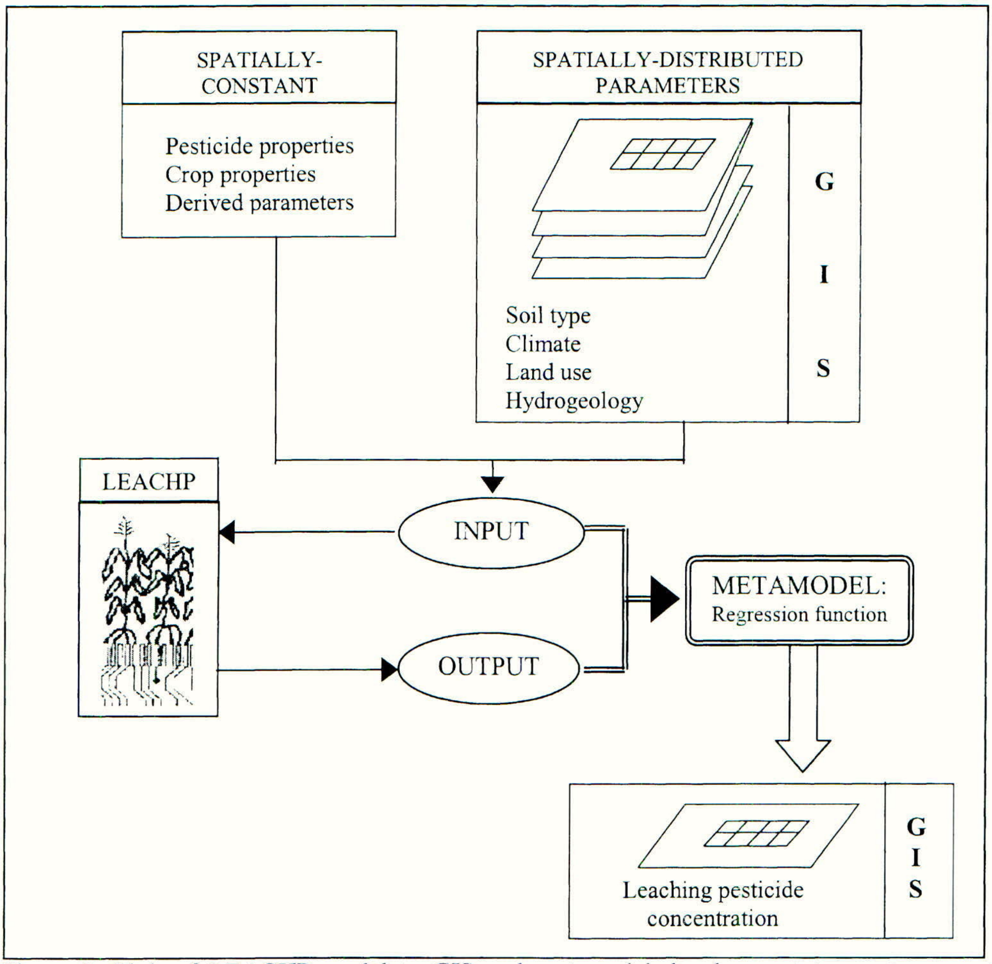

Figure 1. Link of LEACHP model to GIS and metamodel development to create map of pesticide leaching concentrations.

Study area and scenario of application

The approach developed was applied to the plain area in Piacenza Province (Po Valley, Northern Italy) covering approximately 1,100 km^2. The intensive agriculture in the area, associated with the peculiar structure of the aquifer creates a situation where the groundwater risks contamination by pollutants of agricultural origin.

The basic cartography utilised in the study was the soil map at a scale of 1:50.000 defined by 23 different types of soil units: in 40% of the area the soil texture can be classified as silty clay loam, 25.6% is silt loam, 18.5% loam, 6.5% clay and 5.4% silty clay. Soil properties were defined according to 3316 soil profiles distributed across the area. The spatial pattern of the averages of precipitation and temperature (1990-1997) was derived from daily weather data. Evapotranspiration was estimated via the Thornthwaite equation.

Atrazine was the herbicide considered in the simulations (DT_{50} = 44 d; K_{oc} = 118.4 L/kg; K_H = 1.38E-06) applied once per year to a maize crop at a standard dose of 1.9 kg/ha every year).

The LEACHP model was run for 306 soil sampling points selected within each cell (2 x 2 km) of a regular grid (Figure 2). Six years of simulations were performed and as model outputs we considered, according to the FOCUS procedure (FOCUS, 2000) the 80th percentiles of annual average concentration of atrazine leached below 1 meter depth.

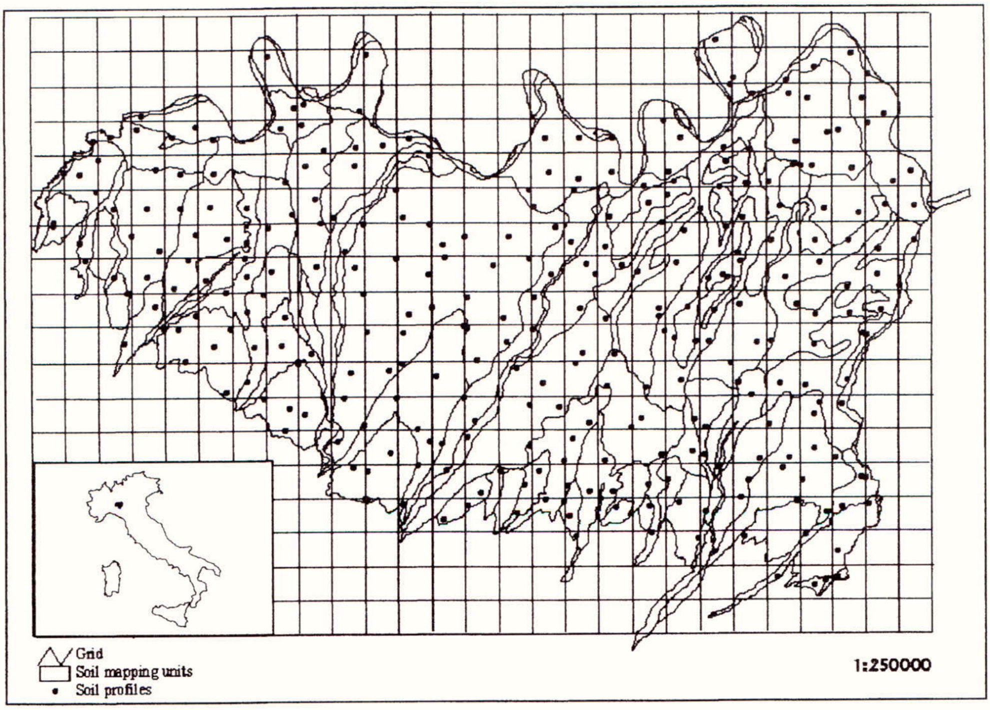

Figure 2. Study area location and selected soil profiles used to perform simulations with the LEACHP model.

Metamodel

Statistical techniques such as stepwise regression procedures are popular methods of searching for good subset models, particularly when the number of independent models is large. In this study the software STATISTIX Version 7.0 (Analytical Software, 2000) was used to summarise the model input-output relationships in order to upscale the concentrations estimated with LEACHP.

RESULTS AND DISCUSSION

A total of 306 values were determined representing the 80th percentile of the atrazine leaching concentration at 1 meter depth in 5 years. The Wilk-Shapiro test for normality suggest a logarithmic transformation of atrazine concentration (LogATR) as the data were not normally distributed. Then, independent variables (clay, bulk density, hydraulic conductivity, silt, organic matter, pH, sand) were analysed statistically with a stepwise regression (Table 1). Soil type has a clear effect on the magnitude of the maximum concentration: clay content and organic matter content are the independent variables with highest correlation with the atrazine leaching concentration.

Table 1. Stepwise regression analysis applied to the LEACHP model output.

STEPWISE REGRESSION OF LogATR

UNFORCED VARIABLES: CLAY BD KS SILT OM PH SAND
VARIABLE(S) DROPPED FROM INITIAL MODEL BECAUSE OF COLLINEARITY: SAND

STEP	R SQ	MSE	P	CLAY	BD	KS	SILT	OM	PH	SAND
1	0.8745	0.08628		A	B	C	D	E	F	.
2	0.8533	0.09169	0.2228	A	B	.	D	E	F	.
3	0.8465	0.08790	0.4926	A	B	.	.	E	F	.
4	0.8272	0.09137	0.2422	A	.	.	.	E	F	.
5	0.8001	0.09813	0.1772	A	.	.	.	E	.	.

RESULTING STEPWISE MODEL

VARIABLE	COEFFICIENT	STD ERROR	STUDENT'S T	P
CONSTANT	2.28951	0.42835	5.34	0.0001
CLAY	-0.08088	0.01525	-5.30	0.0001
OM	-1.21329	0.18444	-6.58	0.0000

CASES INCLUDED	17	R SQUARED	0.8001	MSE	0.09813
MISSING CASES	74	ADJ R SQ	0.7716	SD	0.31326

The resulting regression model ($R^2 = 0.80$) is therefore represented by the following equation:

$$LogATR = 2.28951 - (0.08088*[clay]) - (1.21329*[O.M.])$$

Considering the clay content and the organic matter content of the remaining 3010 soil sampling points, the LEACHP estimated values were extrapolated to the whole study area.

In order to create a raster overlay from the point data, a geostatistical method of interpolation (ordinary kriging) was applied by means of GS^+ software (Gamma Design Software, 1998). The results are displayed by the aid of GIS in a thematic map of the leaching concentration of atrazine at 1 meter depth in the Piacenza plain (Figure 3). It is possible to identify areas of different contamination potentials. Estimated concentrations are less than 0.01 μg/l in almost half of the area whilst in 23% of the area they range between 0.01 and 0.05 μg/l. Largest concentration (18% of the study area) of pesticide are located mainly in the Nord sector, near the Po river and in southern areas characterised by low organic matter soil contents (< 1.5%).

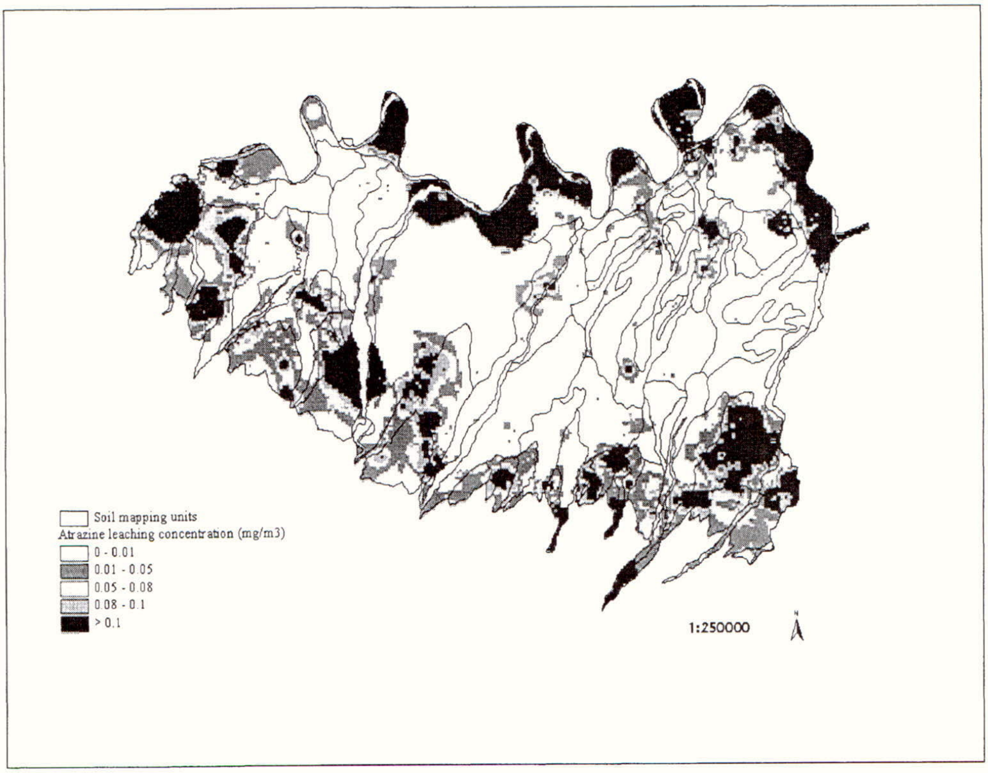

Figure 3. Atrazine leaching concentrations in the Piacenza plain estimated with the LEACHP model.

A validation of the map was carried out with analytical data of pesticide concentrations in drinking water wells. The study area includes 35 wells, which form part of a regional monitoring system. Analytical data for raw water are in good agreement with the map showing that the four wells with atrazine concentrations (average concentrations of seven years of monitoring plan) greater than 0.01 μg/l fall within areas with the largest predicted concentrations.

Results suggest that this approach can be used successfully for evaluating the contamination potential of pesticides in large areas.

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Modelling pesticide input into surface waters in Germany

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ABSTRACT

A GIS decision support system (DSS) is under development for estimating the magnitude and spatial distribution of pesticide losses from non-point sources (surface runoff, tile drainage and spray drift) in Germany. The cumulative annual losses of any active ingredient (a.i.) of known half-life (DT50), adsorption coefficient normalized for organic carbon (Koc) and dosage can be calculated for approximately 400 river basins covering the territory of Germany. Furthermore, the resulting predicted environmental concentration (PEC_{sw}) can be retrieved by relating the daily input of a.i. to the daily discharge of the respective streams. Results are visualized as grid maps with a 1x1 km^2 resolution. Site-specific maps of pesticide losses and PEC frequency distributions provide a basis for regional risk assessment of pesticides.

INTRODUCTION

Pesticide use on agricultural land frequently leads to contamination of non-target areas such as ground water or surface water bodies. An essential condition for an a.i. to meet registration requirements is to rule out contamination of these non-target ecosystems. The "realistic worst-case" is the threshold to determine when a substance can be considered non-toxic for the surrounding ecosystems. The "realistic worst case" is usually determined by laboratory experiments and does not account for the probability of this threshold value being exceeded in its regional and temporal context. The DSS DRIPS follows a probability-based modelling approach on a regional scale by estimating the frequency of a set limit of contamination of a given a.i. and its spatial distribution.

MATERIALS AND METHODS

The modelled non-point sources of pesticide input into surface water bodies are surface runoff, tile drainage and spray drift. DRIPS follows a modular approach, calculating the load or PEC of an a.i. separately.

Runoff

The amount of a.i. to be translocated by runoff water essentially depends on the period of time elapsed between pesticide application and actual occurrence of a runoff-producing rainfall event (Mills & Leonard, 1984). It is assumed that rainfall events of 10 mm in 24 h or larger are sufficient to trigger surface runoff. The 'mean probability of runoff-producing rainfall occurrence' T_n with a given volume h_N and duration in a certain period is determined by the Gumbel-Distribution (Gumbel, 1958).

$$Tn = exp((h_N - u_t) / w_t) \qquad [1]$$

The Gumbel-parameters *u* and *w* are provided by the German Meteorological Service (DWD) with a resolution of 8.5 x 8.5 km^2. Distribution function parameters of 60 min and 24 h duration are currently implemented in the DSS, the latter with separate datasets for summer and winter. According to Mills & Leonard (1984), the probability of a runoff-producing rainfall event *Tn* can also be expressed as a probability density function *f(t)*:

$$f(t) = aT \cdot e^{(-aT \cdot t)} \qquad t \geq 0 \qquad [2]$$

with *aT* as the reciprocal value of *Tn* [cf. 1] and *t* as the time interval between pesticide application and first runoff-producing rainfall event. A seasonal variation factor Vt_i was added to equation [1] to account for the more variable frequency of rainstorm occurrences in the summer season (Auerswald, 1996).

The calculation of the 'runoff volume' Qd_t caused by a runoff-producing rainfall *Pevent* is based on the USSCS's curve-number-method (SCS, 1990). The curve numbers were modified according to Lutz (1984) in order to adapt the SCS-CN-method to Central European conditions.

$$Qd_t = (Pevent - Ia) \cdot Dc + \frac{Dc}{\alpha}\left(e^{-\alpha(Pevent - Ia)} - 1\right) \qquad [3]$$

Land use and hydrological soil group of the land parcel in question determine the drainage coefficient *Dc* (Anderl, 1975; Auerswald & Haider, 1996). Land use data are provided by CORINE land-cover (Statistisches Bundesamt, 1997). The hydrological soil groups were derived from a soil map (BGR, 1996) by Huber *et al.*, (1998) conforming to the SCS-CN methodology.

$$Ia = 0.76 \cdot \left(\frac{10}{Dc} - 10\right) \qquad [4]$$

The initial abstraction *Ia* comprises the processes of interception, initial infiltration rate and surface storage for the time interval passing since the beginning of a rainstorm event until surface runoff starts to occur. Current soil saturation at the time of a rainstorm event is another important factor to be accounted for to calculate the runoff volume. The proportionality coefficient α of Lutz (1984) relates the current soil saturation to seasonal variation.

$$\alpha = P_1 \cdot e^{(-P_2 / WZ)} \cdot e^{(-P_3 / Q_B)} \qquad [5]$$

According to Lutz, the base flow *Qb* of a catchment is the representative factor of its hydrological condition at the beginning of a runoff event. The seasonal variation of the base flow is characterized by week numbers *WZ*. *P1-P3* are calibration factors (Grunwald, 1997). The mean annual precipitation *Pyear* is provided nationwide by the DWD.

The 'pesticide concentration in runoff water' at the beginning of a rainstorm highly depends on the substance's decay as well as the retention capacity of the crop and soil it was applied on. Degradation can be expressed with a first-order decay function (Mills and Leonard, 1984):

$$W(t) = W_{dosage} \cdot e^{(-Bw \cdot t)} \qquad t \geq 0 \qquad [6]$$

where $W(t)$ is the fraction of a pesticide's initial load W_{dosage} left after degrading during the time-interval t since application. Decay is controlled by the breakdown coefficient B_w depending on the a.i.'s half-life $DT50$.

By merging equations [6] and [2], a probability density function can be derived (cf. Mills and Leonard, 1984) for the fraction of the initial load $W(t)$ available on the soil surface for translocation by runoff water of a rainstorm occurring t days after substance application with the probability of $f(t)$ (eq. [2]). Within the DSS DRIPS, mean values (probability = 0.5) of a.i. losses with runoff are assumed (Leonard *et al.*, 1987)

$$W_{0Soil} = 0.5^{\frac{Bw}{aT}} \cdot W_{dosage} \cdot (1 - BG_{i,j}) \qquad [7]$$

Naturally, the full quantity of W_0 is not actually transported by runoff water. A share of it is withheld by the current plant cover of the area the pesticide was applied on. It is assumed that only the portion reaching the soil is available for translocation by runoff. $BG_{i,j}$ is an index representing the degree of soil cover of crop*(j)* in a specific climatic zone at a certain stage of maturity *(i)* (Bach *et al.*, 2000). W_{0Soil} is the runoff-available pesticide load in the surface soil layer.

Only a portion of the runoff-available pesticide load W_{0Soil} is expected to be found in the runoff-suspension during a rainstorm event. That is the fraction of the a.i. subject to desorption processes within the first centimeters of the topsoil. Consequently, the model only calculates pesticide displacement for the liquid phase. Erosion is not taken into account. A semi-empirical approach was adopted from GLEAMS (Leonard *et al.*, 1987) where the soluble amount of the runoff-available pesticide load can be derived by multiplying W_{0Soil} with a desorption-coefficient D_s. An instant balance of an a.i. between the liquid and solid phase is pre-supposed. D_s can be derived empirically from the distribution coefficient Kd, which in turn can be obtained from the linear organic carbon partition coefficient and the content of organic carbon $Corg$ (CREAMS/GLEAMS: Leonard *et al.*, 1987).

Finally, the pesticide concentration of an a.i. in solution $Csolv_{w,t}$ can be calculated from the runoff-available pesticide load W_{0Soil}, the desportion-coefficient D_s and the distribution coefficient Kd. $Csolv_{w,t}$ being the quantity of the initial dosage of an a.i. which has to be expected as surface water input as a result of a runoff-producing rainstorm event.

$$C_{solvwt} = \frac{W_{0Soil} \cdot D_s}{1 + D_s \cdot Kd} \qquad [8]$$

2.2 Leaching

Germany's registration authorities make use of the model PELMO by Klein *et al.* (1997) for assessing the risk of a.i. displacement via leaching. To conform to registration standards, PELMO was adopted in DRIPS as the model of choice to estimate the quantity of pesticides transported by leaching water. PELMO is used to simulate the displacement of an a.i. to 0.8 m depth. At that depth, the leachate is expected to enter a tile drainage system - if installed on the land – or be subject to further vertical translocation. In the latter case, the pesticide ultimately reaches the ground water body, if it does not fully degrade along the way. The input of pesticides into surface waters from the ground water body is considered to be negligible in Germany (Bach *et al.*, 2000). Hence, pesticide input via leaching is only calculated for drained areas. A grid cell map of Germany's drained areas is provided by Behrendt *et al* (1999). DRIPS estimates the site-specific input $L(leach.)_{w,i,j}$ of an a.i. dosage W applied on date (i) and crop (j) via a tile drainage system.

$$L(leach.)_{w,i,j} = W_{i,j,} \cdot (1 - BG_{i,j}) \cdot \delta(PELMO)_w \qquad [9]$$

In the same manner as for the runoff path, it is presupposed that only that amount of an a.i. is transported in the leachate, which is not subject to foliage-interception but reaches the soil. Since PELMO does not consider interception, BG is introduced as an index of the degree of soil cover of crop (j) in a specific climatic zone at a certain stage of maturity(i). $\delta(PELMO)_w$ is the fraction of the initial dose of an a.i. found in the leachate at 0.8 m depth. The solution is expected to enter a tile drain at that depth leading towards a surface water body nearby.

2.3 Spray drift

Surface water input of a sprayed a.i. is expected via direct drift, for the fraction of the substance not reaching the target area but being blown into an adjacent stream. Generally, a.i. loss by drift is significantly higher for fruit- or grapevine plantations than for field crops. This is mainly due to different spraying-techniques, like the use of boom sprayers in field crops and air blast sprayers in grapevine plantations (Ganzelmeier *et al.*, 1995). DRIPS uses the drift tables published by Germany's Federal Biological Research Center for Agriculture and Forestry (BBA) as a basis for estimating the fraction of an a.i. displaced by spray drift. The tables are also used by registration authorities to set up spraying-distance requirements for pesticides. Different tables are available for 95th, 70th and 50th percentiles providing separate spray drift values $BBA\text{-}Tab(Dist)_w$ for fruit grapevine and field crops each for two phenological zones and for specific proximities of surface water and site of application.

$$L(drift)_{w,i,j,} = BBA\text{-}Tab(dist)_w \cdot W_{i,j,} \cdot A \backslash G \cdot Gd_r \cdot Gbr \qquad [10]$$

where $L(Drift)_{w,i,}$ is the site-specific input of a.i. W via spray drift after application at date(i) in crop(j). $A \backslash G$ is a correction factor for the cropland/pasture ratio adjacent to rivers. In DRIPS $A \backslash G$ is set to 0.4 for cropland and 1.0 for fruit- and grapevine plantations (Bach *et al.*, 2000). The mean drainage density of the river network Gd_r was derived from the Hydrological Atlas of Germany (HAD) by Huber *et al.* (1998). It is available within DRIPS as a grid map to judge the probability of an a.i. reaching a surface water body via drift. The amount of a.i. input also depends on the width of the river Gb. Larger water bodies are susceptible to higher amounts of deposition. However, most larger streams have adequate buffer zones shielding a.i. input to some extent. Unshielded small ditches are frequently found in agriculturally used areas prone to receive frequent deposition. In DRIPS Gb is set to 0.5 m for 1st order streams (definition of Strahler, 1957) and 3 m for 2nd order and higher.

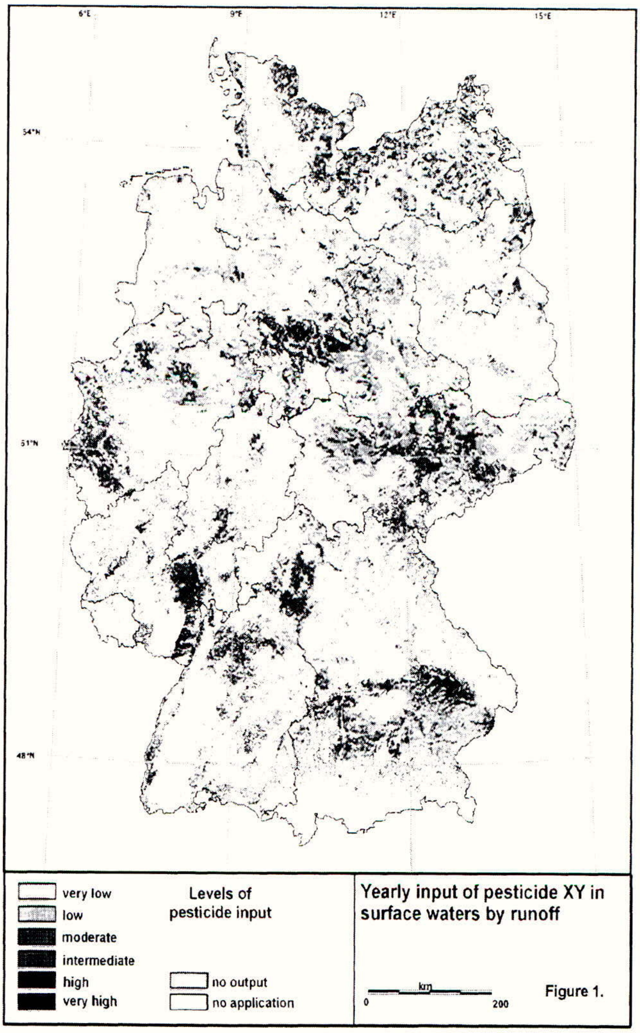
2.4 PEC

The model approaches described for runoff, drainage and spray drift estimate the expected load of pesticides input into surface water bodies for a specific region and time. DRIPS will be fitted with a further module to estimate the initial predicted environmental concentration (PEC_{SW}). The module will link the three pathways calculating the a.i.'s load with hydrological data such as rivermorphology and flow duration. The basic river network to be used is provided by Behrendt *et al.* (1999). The network will be classified into approximately six regions *(r)* of similar drainage density and rivernet-morphology. Also, all surface water bodies will be classified *(g)* according to their volume of discharge. Significant combinations of both classes *(r)* and *(g)* such as drainage density of 2nd order streams in a certain region will be used as model variables. An evaluation of gauging station data will produce discharge values for every class on a daily basis. The ratio of the mean daily input (E) of an a.i. via runoff, drainage and spray drift into various types of surface water bodies characterized by their daily discharge (Q) yields the predicted environmental concentration of the respective surface water body.

$$PEC_{sw} = E/Q \qquad [11]$$

RESULTS AND DISCUSSION

Figure 1. Map of results from DRIPS



The model described above will be fully integrated into a GIS-shell with an easy to use graphical interface. The DSS DRIPS is set up as a user-friendly risk assessment tool for estimating the PEC_{sw} of a.i. in surface water bodies. Results will be available with fairly high temporal (eg. daily discharges) and spatial (1x1 km^2) resolution. The DSS offers a time- and cost-effective method to assess the probability of pesticide contamination of surface waters and the resulting initial concentration of the a.i. in surface water bodies. Relatively few parameters have to be specified by the user, such as dosage, DT50, Koc, crop and date of application. Spatially discriminated maps are produced as model results visualizing the hazard potential for the territory of Germany with its varying soil and climatic conditions. Authorities could use these maps as a basis to encourage field campaigns for specific substances at sites where high contamination is expected.

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