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Biases in the spatial estimation of pesticide loss to groundwater

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Abstract – Prediction of pesticide fate in soils is highly sensitive to parameters describing sorption and degradation processes, namely the K_{oc} partitioning coefficient between the soil solution and organic carbon fraction and the half-life DT_{50} for degradation. This paper explores the impact of getting K_{oc} and DT_{50} values either from databases or from site-specific measurements on the predicted fate of atrazine, isoproturon and metamitron on the catchment scale. Pesticide fate on the scale of the Bruyères-et-Montbérault catchment, France, was predicted using the SEAMS software that couples a one-dimensional local-scale model of pesticide fate to a geographic information system. The results show that the use of database average values for K_{oc} and DT_{50} underestimates the average risk of pesticide leaching calculated from site-specific K_{oc} and DT_{50} values, whereas maximised risk scenarios based on extreme K_{oc} and DT_{50} values may be overestimated when using database values. Whenever available, site-specific data should be preferred to limit bias in pesticide leaching risk assessments on the catchment scale.

pesticide fate / herbicide / spatial variability / soil / environmental risk assessment

1. INTRODUCTION

Pesticides constitute a major environmental problem. Their widespread use in agriculture and other human activities has led to the contamination of numerous surface and groundwater resources throughout the world (Leistra and Boesten, 1989; Kolpin et al., 2000; IFEN, 2004). Environmental protection and catchment management agencies, regulatory authorities, pesticide registration offices and farmers are developing and/or using tools for the prediction of pesticide concentration levels in the various compartments of the environment (FOCUS, 1995). Concerning groundwaters, prediction of concentration levels is generally done by using a one-dimensional model describing the fate of pesticides in soil on the local scale (FOCUS, 2000; Dubus et al., 2002), coupled with a Geographic Information System (GIS) that is able to store geographically-referenced input data as well as mapping output modelling results (Hornsby, 1992; Sunday Tim, 1996; Corwin et al., 1997).

Predicted groundwater concentrations need to be accompanied by some estimation of their uncertainty (Vermeire and van der Zandt, 1995; Dubus et al., 2003b). Sensitivity analyses of pesticide fate models have shown predicted concentrations to be highly sensitive to input values, especially those describing sorption and degradation processes (Boesten, 1991; Dubus et al., 2003a). Sorption in soils is often described in pesticide

fate models by a linear instantaneous partitioning between the soil solution and the organic carbon fraction of the soil solid phase, and characterised by the partition coefficient K_{oc} , in mL/g, where oc stands for “organic carbon” (Hamaker et Thompson, 1972). Degradation is generally modelled by a first-order kinetics, which can be characterised by the half-life, or DT_{50} (in days, where DT stands for “degradation time” and 50 for “50% of the initial pesticide concentration”), of the pesticide (Beulke and Brown, 2001). These pesticide fate parameters should be measured in the various soils found in the geographic zone where the risk assessment is to be conducted. Pesticide partition coefficients and half-lives are known to be spatially variable (Elabd et al., 1986; Rao et al., 1986) and this variability should be quantified and accounted for in the risk assessment procedure. However, due to the cost of obtaining local references for such data, risk assessments are often based on generic registration data or international or national databases. These include values that have generally been measured on a variety of soils scattered over the world, but mostly in the USA and Europe.

Our objective was to test the feasibility of making sound risk assessment of groundwater contamination by pesticides on the local catchment scale using pesticide sorption and degradation databases. These “generic” assessments will be compared with others made using local information on K_{oc} and DT_{50} and their variability on the catchment scale that has been previously

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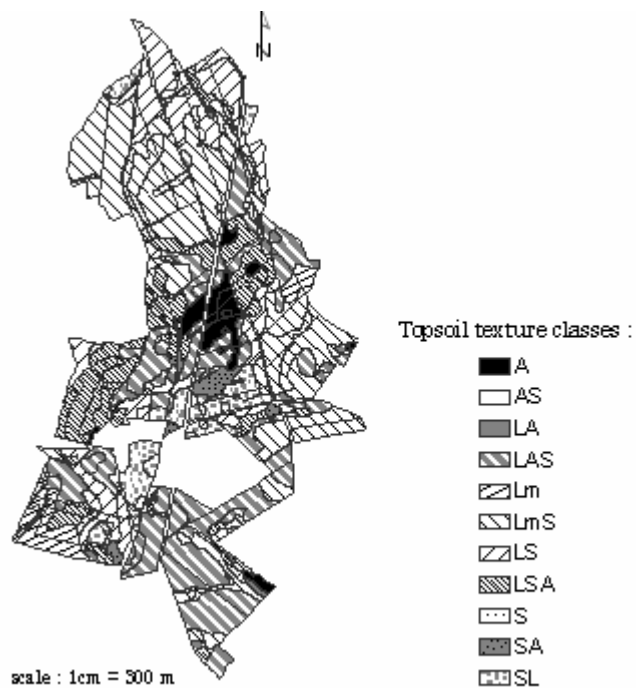


Figure 1. Map of the topsoil texture of the Bruyères-et-Montbérault catchment. Soil texture is highly variable within the catchment due to the diversity of subsoil materials (sands, loams, clays, marlstones, limestones).

obtained (Coquet and Barriuso, 2002; Charnay et al., 2005). Some general recommendations for local-scale risk assessment will then be drawn.

2. MATERIALS AND METHODS

2.1. The catchment

The catchment used for this study is located in the North of France (Aisne Département, Picardie Region) in Bruyères-et-Montbérault. Its surface area is 187 ha and includes 135 ha of cultivated land composed of 31 agricultural fields. Three farmers cultivate the fields under the same type of intensive cropping system that includes winter wheat, barley, sugar beet, rape seed and pea. Most of the fields are heterogeneous from a pedological point of view due to a high variability in parent material (Fig. 1) (Beaudoin et al., 2004). Textures range from sand to clay but the majority of the soils are loamy due the presence of partially eroded loess deposits. Twenty-one soil typological units were mapped on the 1/7500 scale (Fig. 1). Crossing the various soil mapping units with the 31 agricultural fields resulted in 190 SIMulation Units (SIMUs). Each SIMU may be regarded as homogeneous from the point of view of input data for pesticide fate modelling. The soils have a good hydraulic conductivity and runoff was very limited within the catchment. The soil water drained at the bottom of the crop root

zones recharges an unconfined aquifer below the catchment. This aquifer is in turn drained by numerous springs, two of which are currently used as drinking water supplies. Traces of atrazine found in some springs have led to concern about the vulnerability of the catchment groundwater to pesticide contamination.

2.2. The risk assessment tool

A coupled GIS-model tool was used for the risk assessment of groundwater contamination by the agricultural pesticides used in the catchment. We used SEAMS (Soil Environmental Agricultural Management System) (Hoogeweg and Hornsby, 1999), which has been developed by the University of Florida in Gainesville and is an integration of CMLS96B (Nofzinger and Hornsby, 1986) into ArcView[®] 3.2 (ESRI, Redlands, California). According to Corwin et al. (1997), the coupling between CMLS96B and ArcView[®] is of the “tight” type, which means that both the model and the GIS share a common user interface and that data exchange between the model and the GIS is transparent to the user.

CMLS96B is one of the simplest models for simulating pesticide fate in soils (Calvet, 1995). It is a one-dimensional functional model based on a tipping-buckets representation of water flow. This representation implies that CMLS96B cannot account for hydrodynamic dispersion during transport or for upward water flows such as capillary rises. Physicochemical properties are assumed to be homogeneous within each horizon. Sorption processes are assumed to respect an instantaneous, linear and reversible equilibrium. Pesticide degradation is considered to be identical in all the horizons of the soil profile and to follow the same first-order kinetics. Time-dependent sorption or water content and temperature effects on degradation rates are not included in CMLS96B. CMLS96B simulates the advance of the pesticide pulse within the soil profile and SEAMS records the following outputs from CMLS96B: the pesticide mass (mg/ha) that reaches a user-defined “control depth”, for each SIMU; the travelling time (days) of the pesticide down to the “control depth”; and the “average load”, which is the spatial mean of the pesticide mass that reaches the “control depth” on the catchment scale.

SEAMS manages climatic input to CMLS96B in a stochastic way by using the weather generator WGEN (Richardson and Wright, 1984). This tool produces simulated climatic series of unlimited duration for a given site based on the statistical characteristics of the local climate using Markov chain simulation. Up to 15 years of climatic data may be generated by WGEN for a SEAMS simulation. We here define one “simulation” as the one-dimensional transport modelling of a specific herbicide down to the control depth within each of the SIMUs composing the catchment. A simulation may last up to 15 years depending on the travelling time and degradation rate of the pesticide. SEAMS stops a simulation either when the pesticide reaches the control depth or when the totality of the pesticide has been degraded. Simulations have to be repeated for the same scenario to account for the variability of the climate generated by WGEN. Up to 650 simulations may be done by SEAMS to account for climate variability as recommended by Dubus and Janssen (2003). We set the number of simulations at the maximum allowed by SEAMS because of the highly non-linear

Table I. Description of K_{oc} and DT_{50} data sets for use in the risk assessment scenarios.

	Database values							Measured values					
	mean	nb. obs.	min	max	P20	P80	mean	nb. obs.	min	max	P20	P80	
K_{oc} (mL·g ⁻¹)	Atrazine	123	13	38	174	88	157	63	51	52	83	55	72
	Isoproturon	155	2	80	230	–	–	66	51	52	90	58	75
	Metamitron	168	1	–	–	–	–	75	51	48	95	65	86
DT_{50} (days)	Atrazine	69	13	18	120	45	110	32	51	12	39	27	35
	Isoproturon	29	6	12	45	21	32	13	14	5	31	9	15
	Metamitron	28	1	–	–	–	–	17	14	14	22	15	18

P20: 20th percentile, P80: 80th percentile.

response of CMLS96B outputs to climate variations. We here define a “prediction” as the results of the 650 simulations done to assess pesticide dissipation for a particular scenario. In the following, we will note as m_{SIMU} , or “local load”, the arithmetic mean of all simulations for a particular SIMU within a particular prediction, and se_{SIMU} the standard error of the mean of all simulations for a particular SIMU and prediction. The spatial mean, or “average load”, of all m_{SIMU} values for a particular prediction will be noted as M_{WS} and the standard error of this spatial mean (SE_{WS}) will be noted as SE_{WS} . In this way, we can consider that the average value of se_{SIMU} on the catchment scale is a characterisation of the temporal variability of the risk due to climatic variation, whereas SE_{WS} characterises the spatial component of risk variability.

2.3. Input data

SEAMS requires input data on climate, agricultural practices, soils and pesticides. No climatic data were directly measured within the catchment. Climatic data were taken from the meteorological station of St Quentin-Roupy (Aisne Département) located 56 km from Bruyères-et-Montbérault. Data on maximum and minimum daily temperatures, daily solar radiation and daily rainfall from the 01/01/1986 to 31/12/1998 period were used to derive the statistical parameters for WGEN. Agricultural data were provided by the INRA Agronomy Station of Laon. They included the maximum rooting depth, the soil volumetric water content below which the plant suffers from water stress and the crop coefficients at the various development stages of each crop cultivated in the catchment. Soil data were also provided by the INRA Agronomy Station of Laon. Each horizon encountered in the soils of the catchment was documented by its depth boundaries, organic carbon content, bulk density, water contents at field capacity and wilting point, porosity and texture. Pesticide data included two parameters: the half-life, DT_{50} (days), of the pesticide and its sorption coefficient normalised by the organic carbon content, K_{oc} (mL/g). Data were either taken from available databases on sorption and degradation properties of pesticides (Dabène et al., 1995; Hornsby et al., 1996) or calculated from measured laboratory data (Coquet and Barriuso, 2002; Charnay et al., 2005).

2.4. Risk assessment scenarios

An agricultural survey of the catchment showed that up to 86 different pesticides have been used from 1989 to 1997, with the largest quantities being herbicides. From among them, we selected three herbicides as being representative of the various crops cultivated in the catchment: metamitron, used on sugar beet, ranked fourth among all the pesticides listed in the decreasing order of their accumulated load on the catchment scale during the 1989–1997 period, with a total of 484 kg of active ingredient; isoproturon, used on cereals, ranked eighth with a total of 228 kg; and atrazine ranked only thirtieth with a total of 25 kg due to its limited use on occasional maize fields but was included because it had been the only pesticide detected in spring waters during annual surveys. SEAMS does not allow for simulation of crop successions. Therefore, risk assessments were done separately for each herbicide, considering the monoculture in the whole catchment for all the duration of each prediction.

Risk assessments need to account for the variability of input data. By construction, SEAMS accounts for climate variability through a stochastic generation of climate. All input data may be subject to variability. However, as most pesticide fate models are mostly sensitive to sorption and degradation parameters, we limited our analyses to K_{oc} and DT_{50} variability impacts. Preliminary trials showed that the SEAMS results were indeed most sensitive to these two parameters. Based on the variability of the K_{oc} and DT_{50} parameters in the literature or measurement databases, we designed two scenarios for the risk assessment of pesticide leaching in the Bruyères-et-Montbérault catchment.

We first designed a scenario that could account for an average leaching risk. In this scenario, the arithmetic averages of all the K_{oc} and DT_{50} values either found in the databases or measured within the catchment were used (Tab. I). K_{oc} and DT_{50} literature databases were those from Hornsby et al. (1996) for atrazine, and from Dabène et al. (1995) for isoproturon and metamitron, which are not included in the Hornsby et al. database. The Hornsby et al. database includes 13 K_{oc} and 13 DT_{50} values for atrazine. The Dabène et al. database includes 6 DT_{50} values for isoproturon but only 2 extreme values for K_{oc} . Only one value of K_{oc} and DT_{50} were available for metamitron. These two values were taken as averages for metamitron, and

Table II. Simulation parameters used for the three herbicides in all risk assessment scenarios.

Herbicide	Atrazine	Isoproturon	Metamitron
Crop	corn	wheat	beet
Application rate (kg/ha)	0.95	1	8.8
Application dates (year n)	1–2 May	15–16 March	1–2 June
Root depth (m)	1.2	1.3	1.5
Control depth (m)	0.6	0.6	0.6
Number of simulations over 15 years	650	650	650

Table III. Prediction results: average load M_{WS} values in mg/ha. Standard error (SE_{WS}) is given in parentheses. Generic scenarios based on literature K_{oc} and DT_{50} values underestimate the average risk of pesticide loss to groundwater compared with site-specific scenarios using K_{oc} and DT_{50} measurements on the catchment scale.

	Average risk		Maximised risk	
	generic scenario	site-specific scenario	generic scenario	site-specific scenario
Atrazine	0.19 (2.40)	0.417 (4.21)	57.9 (273.6)	2.58 (20.71)
Isoproturon	0	0.000013 (0.000033)	0.012 (0.037)	0.089 (0.59)
Metamitron	0	0.0015 (0.025)	–	0.74 (6.88)

an average K_{oc} was calculated as the mean of the two available values for isoproturon. Fifty-one measured values were available for atrazine, isoproturon and metamitron K_{oc} s (Coquet and Barriuso, 2002) (Tab. I), as well as for atrazine DT_{50} , but only 14 measured DT_{50} values were available for isoproturon and metamitron (Charnay et al., 2005).

Secondly, we designed a “worst-case” scenario that would maximise the leaching risk by considering a low degradation and a low sorption of the pesticide by the soils. For this scenario, we used two different approaches, whether the database was from on-site measured data or from literature surveys. When using literature databases, we used the 20th percentile for K_{oc} and 80th percentile for DT_{50} in order to exclude outliers. As only 2 values were available for isoproturon K_{oc} , we used the lowest value for the maximised risk scenario. Of course, no worst-case scenario could be constructed for metamitron from the Dabène et al. (1995) database as only one value was available for K_{oc} and DT_{50} . For the maximised risk scenario based on measured data, we used the extreme values of the data sets because they were indeed real values encountered in the Bruyères-et-Montbérault catchment and relevant for the evaluation of a worst-case situation on the catchment scale. Parameters related to soil properties and agricultural practices were kept constant for all risk assessments (Tab. II). In the following, we will refer to the scenarios based on literature databases as “generic” scenarios, whereas those based on the available measurements will be designated as “site-specific” scenarios.

3. RESULTS AND DISCUSSION

3.1. Average risk scenarios

For all three herbicides, the generic average risk scenario underestimates the real average leaching risk as estimated by the site-specific scenario (Tab. III). The average load M_{WS} for

atrazine estimated from literature databases is half that estimated using on-site data. The groundwater contamination risk estimated from the pesticide residual mass that reaches the 60-cm control depth decreases in the order: atrazine > metamitron > isoproturon. No isoproturon or metamitron reaches the 60-cm control depth in generic scenarios, whereas 0.013 and 1.52 $\mu\text{g}/\text{ha}$ of isoproturon and metamitron were simulated at the 60-cm control depth for site-specific scenarios.

Pesticide load on the SIMU scale, or “local load”, is highly variable within the catchment as denoted by coefficients of variation (CVs) of m_{SIMU} , calculated as the ratio of SE_{WS} to M_{WS} (Tab. III), in the order of magnitude of 1000% for both types of scenarios. Values of m_{SIMU} range from 0 to a maximum of 70.6, 0.0001 and 0.43 mg/ha for atrazine, isoproturon and metamitron, respectively, for the site-specific scenarios. The maximum local load for atrazine was only 40.5 mg/ha for the generic scenario, which means that the generic scenario also underestimates the local average leaching risk within the catchment.

The location of the maximum local load within the catchment is always the same regardless of the pesticide or the type of scenario (Fig. 2): it is a small SIMU located at the top part of the catchment with very low soil organic matter content (5.5 g C/kg dry soil). However, the pattern of the leaching risk within the catchment varies greatly according to the type of scenario (Fig. 2). Some SIMUs, in which all atrazine is degraded before reaching the control depth when considering in-situ data, have a non-zero local load when using literature databases, and vice versa.

3.2. Maximised risk scenarios

In contrast to the average risk assessment, generic scenarios overestimate the maximised leaching risk of atrazine within the catchment when compared with site-specific scenarios (Tab. III).

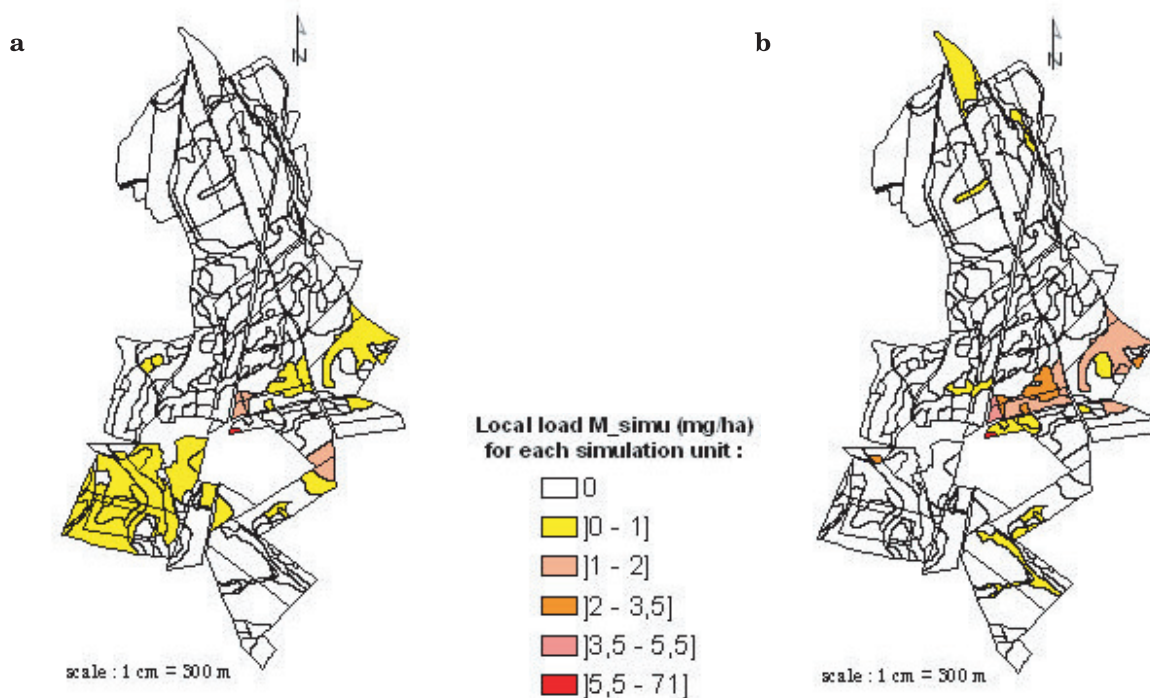


Figure 2. Prediction results for the atrazine average risk scenario: (a) with K_{oc} and DT_{50} database values (Horsnby et al., 1996); (b) with K_{oc} and DT_{50} measured values. The catchment-scale average load, M_{WS} , is larger for prediction b than for prediction a. Some simulation units have non-zero local loads for prediction a but not for prediction b, and vice versa. The local load level for some simulation units is also variable between the two predictions a and b.

The average load, M_{WS} , is 22 times larger when estimated from the literature database percentiles than when estimated from the extreme on-site values of K_{oc} and DT_{50} for atrazine, but 5 times lower for isoproturon. From the atrazine results, it seems that using the 20-percentile value for K_{oc} and the 80-percentile value for DT_{50} is a reasonably conservative approach to the estimation of the maximum risk of pesticide leaching on the catchment scale. However, such a strategy does not hold for isoproturon even though the database minimum K_{oc} value was used in place of the unavailable 20-percentile value. This is due to the fact that this database minimum K_{oc} value was indeed larger than the minimum K_{oc} value measured within the catchment (Tab. I). Atrazine M_{WS} at the 60-cm depth was equivalent to a soil solution concentration of 0.52 $\mu\text{g/L}$ for the generic scenario, and 0.018 $\mu\text{g/L}$, for the site-specific scenario.

As for average risk scenarios, local loads are variable within the catchment. Coefficients of variation of m_{SIMU} are around 400% for generic scenarios and vary between 600 and 1000% for site-specific scenarios (Tab. III). When using site-specific scenarios, maximum local load values are 330, 8.8 and 110 mg/ha, which represent 0.035, 0.0009 and 0.011% of the applied dose for atrazine, isoproturon and metatitron, respectively. When using generic scenarios, maximum local loads increase to 3800 and 14 mg/ha; that is, 0.4 and 0.0015% of the applied dose, for atrazine and isoproturon. The location of this maximum local load within the catchment is the same for all pesticides and is identical to that recorded by the average risk scenarios.

The leaching pattern of atrazine on the catchment scale is quite consistent between the generic and site-specific scenarios (Fig. 3). When compared with the site-specific scenario, the generic scenario appears to be a translation of the simulated loads towards higher values, with a larger proportion of the catchment having non-zero m_{SIMU} values. On the contrary, leaching patterns of isoproturon (Fig. 4) vary significantly between the site-specific and generic scenarios. A slightly larger zone of the catchment has a zero local load for the generic scenario compared with the site-specific one, especially in the northern part of the catchment, whereas there is a high local load zone at the southwestern end of the catchment.

Average se_{SIMU} values were 14.9, 0.95 and 4 mg/ha for atrazine, isoproturon and metatitron, respectively, using site-specific scenarios. Comparing with the SE_{WS} values from Table III, we find that the temporal variability of simulated loads due to climate variations (given by the se_{SIMU} values) was slightly lower than the catchment-scale spatial variability (given by the SE_{WS} values), except for isoproturon. Similar types of results were obtained by Jury and Gruber (1989).

Passing from an average risk to a maximised risk assessment naturally increases the average load. Atrazine M_{WS} is multiplied by 300 when considering generic scenarios, but only by 6 when considering site-specific scenarios. Still using site-specific scenarios, M_{WS} increases seven thousand-fold and five hundred-fold for isoproturon and metatitron, respectively. We see here that the lower the leaching risk, the higher the sensitivity of the leaching level to the K_{oc} and DT_{50} values (Boesten,

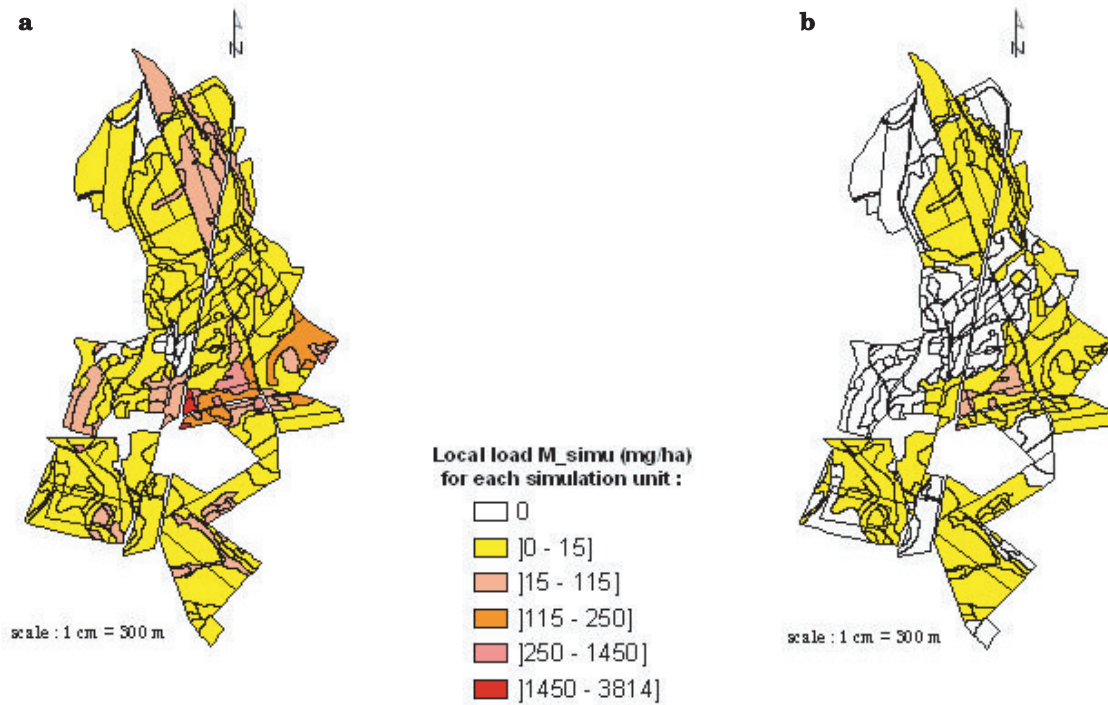


Figure 3. Prediction results for the atrazine maximised risk scenario: (a) with K_{oc} and DT_{50} database values (Hornsby et al., 1996); (b) with K_{oc} and DT_{50} measured values. The catchment-scale average load, M_{WS} , is larger for prediction a than for prediction b. The use of the generic scenario tends to overestimate average and local loads.

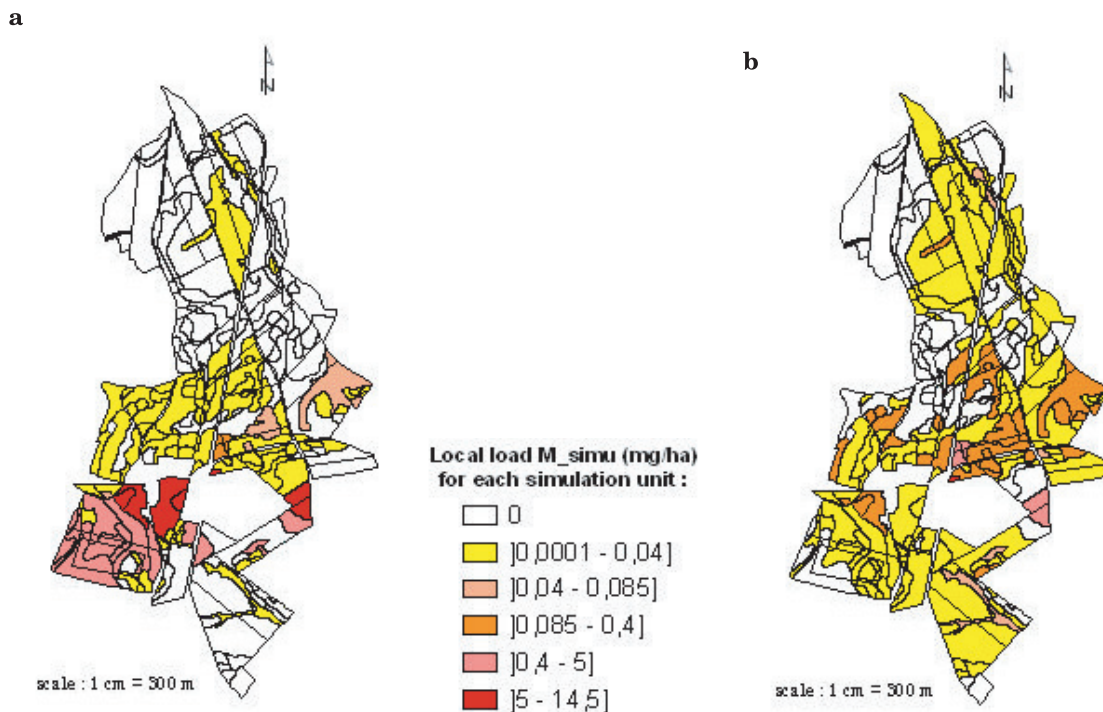


Figure 4. Prediction results for the isoproturon maximised risk scenario: (a) with K_{oc} and DT_{50} database values (Dabène et al., 1995); (b) with K_{oc} and DT_{50} measured values. Although the average load M_{WS} is larger for prediction b than for prediction a, specific simulation units (especially in the south-west of the catchment) present a much larger local load in prediction a than in prediction b: the local risk of isoproturon loss toward groundwater is largely dependent on the K_{oc} and DT_{50} information source.

Table IV. Prediction results to estimate the effect of K_{oc} and DT_{50} variability on leaching risk assessment: average load M_{WS} in mg/ha. Standard error (SE_{WS}) is given in parentheses. Average load is generally more sensitive to DT_{50} than to K_{oc} variations.

	Generic scenario				Site-specific scenario			
	K_{oc} min	K_{oc} max	DT_{50} max	DT_{50} min	K_{oc} min	K_{oc} max	DT_{50} max	DT_{50} min
Atrazine	3.74 (38.17)	0.05 (0.70)	9.08 (54.90)	0.006 (0.09)	0.920 (7.33)	0.05 (0.83)	0.916 (9.76)	0.00007 (0.0009)
Isoproturon	0.016 (0.071)	0	0.000013 (0.00003)	0	0.000003 (0.00005)	0	0.051 (0.250)	0
Metamitron	–	–	–	–	0.098 (0.969)	0.00008 (0.0014)	0.0225 (0.373)	0.00005 (0.00084)

1991). Finally, it is important to note that the average risk scenario based on literature data does not cover the real site-specific “worst-case” scenario (Tab. III).

3.3. Sensitivity to input data variability

The sensitivity of the leaching risk to climate variability is inherently considered by SEAMS. Based on average se_{SIMU} values, we estimated that the variability due to climate was of the same order of magnitude as that due to variations in soil properties within the catchment. We also showed through the comparison of average and maximised risk or generic and site-specific scenarios that the leaching risk was highly sensitive to K_{oc} and DT_{50} values.

We further explored this variability by considering K_{oc} and DT_{50} variations one at a time and taking the extreme values of either the field data set or the literature database (Tab. IV). The main result from this analysis is that, generally, the variability of DT_{50} has a larger impact on risk assessment than the variability of K_{oc} . Taking the extreme field K_{oc} values together with a mean field DT_{50} resulted in an eighteen-fold change in M_{WS} for atrazine, whereas using the extreme field DT_{50} values and mean K_{oc} resulted in a thirteen thousand-fold change in M_{WS} . When considering generic data, M_{WS} was modified by a factor of 75 due to K_{oc} variation, but by a factor of 1500 due to DT_{50} variation (Tab. IV).

The same type of result was also obtained for isoproturon with site-specific data, whereas M_{WS} was found to be more sensitive to K_{oc} variation in the literature database than to DT_{50} variation. This result may be attributed to the limited range of DT_{50} variation found in the Dabène et al. database, compared with the DT_{50} variation for atrazine found in the Hornsby database (Tab. I). Metamitron M_{WS} was found to be highly sensitive to K_{oc} field variation, and as much as to DT_{50} field variation. However, the range of metamitron DT_{50} values measured in the catchment was particularly low, when compared with that of atrazine or isoproturon (Tab. I).

3.4. SEAMS limitations

Although SEAMS comes as a useful integrated tool for pesticide leaching risk assessment, it is subject to some drawbacks or limitations. Some of them are related to the pesticide fate model CMLS96B. The most important one is probably the fact that degradation rates are similar in the surface and subsoil. Yet, degradation rates are known to decrease dramatically with depth (Di et al., 1998; Charnay et al., 2005). As a consequence, pesticide degradation in the soil profile was probably overes-

timated. In our risk assessment scenarios, no pesticide reached the 1-m depth, which is generally the reference depth considered in groundwater contamination risk assessments (FOCUS, 2000). As a consequence, we chose to displace the SEAMS control depth to 60 cm in order to get proper relative risk assessments, considering that no degradation was occurring between the 60- and 100-cm depths. Other models could have been used in place of CMLS96B for the purpose of simulating the local fate of the pesticides. We used CMLS96B as a component of SEAMS, which was the only GIS-coupled pesticide fate model tool at hand freely available when we started our work. However, other tools such as GeoPEARL (Tiktak et al., 2003) could be used for similar purposes.

Another limitation was related to the maximum number of simulations that could be performed within the same prediction. Preliminary tests showed that the average load M_{WS} was highly variable between repeated predictions of the same scenario when using less than 500 simulations per prediction. Therefore, the number of simulations was set to the maximum allowed by SEAMS, 650, in all predictions. Yet, some variability of M_{WS} could still be detected, which means that the prediction associated with a particular scenario was not strictly repeatable. The standard error of the mean for 8 successive predictions of the maximised risk scenarios was 1.01, 0.14 and 0.61 mg/ha for atrazine, isoproturon and metamitron, respectively, which is less than the temporal and spatial variability as judged from se_{SIMU} mean values and SE_{WS} values (Tabs. III, IV). Dubus and Janssen (2003) showed that the number of simulations per prediction should be at least 5000 in order to achieve a sufficient stability in the stochastic modelling results.

3.5. Recommendations for pesticide leaching risk assessment

Some basic recommendations can be made in the light of the results presented here.

1. The use of average values from literature databases is not satisfactory for the purpose of catchment-scale risk assessment. Whenever data on the spatial variability of sorption and degradation processes in the soils of the catchment are available (or in soils known to be similar to them), that information should be used preferentially.

2. When no local data is available, the use of database 20 and 80 percentiles or, by default, extreme values for K_{oc} and DT_{50} should be used. Such values seem to be conservative and may be recommended for risk assessments.

3. Databases on K_{oc} and DT_{50} should include at least average (or median) and extreme values for all pesticides in current use.

However, it is difficult to know to what extent such recommendations will be generally applicable to the various catchment situations. Additional analyses such as the one presented here are needed before being able to reach the goal of making reasonably sound risk assessments.

4. CONCLUSIONS

We showed that pesticide leaching risk assessments were crucially dependent on the available K_{oc} and DT_{50} information. In our case study on the fate of atrazine, isoproturon and met-amitron, the average risk evaluated using mean K_{oc} and DT_{50} values extracted from literature databases was seriously underestimated when compared with that made by using field-measured data. Using 20-percentile and 80-percentile literature database values for K_{oc} and DT_{50} overestimated the maximised risk as estimated from the extreme field K_{oc} and DT_{50} values and may be regarded as a conservative approach. A simplified sensitivity analysis showed that DT_{50} variability had a larger impact on risk assessment than K_{oc} variability for all three herbicides.

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