"Assessing pesticide leaching at the regional scale : a case study for atrazine in the Dyle catchment/"

Leterme, Bertrand

ABSTRACT

The overall objective of this thesis is to better understand and assess pesticide leaching at the regional scale, using both the analysis of monitoring data and spatially distributed modelling. Atrazine contamination of the Brusselian aquifer (central Belgium) is poorly understood. Considerable uncertainty surrounds whether the pollution is agricultural or non-agricultural in origin. The spatial and temporal covariance of atrazine concentrations was studied by fitting semivariogram models to monitoring data. Correlation ranges were found to be 600 metres and 600-700 days. A non-parametric one-way ANOVA found a strong relationship between mean concentrations and land use, whilst other environmental variables were found to be less important. Higher levels of pollution were detected in areas dominated by urban land use suggesting that atrazine residues in groundwater resulted from non-agricultural applications. Modelling pesticide leaching at the regional scale (Dyle catchment) was used to assess groundwater vulnerability. Different approaches to process soil information were tested with both a linear (modified Attenuation Factor) and a non-linear (GeoPEARL) leaching model. The CI (calculate first, interpolate later) and IC (interpolate first, calculate later) approaches were identical for the linear model, but differences in the amount of leaching were found for the non-linear model. The CI approach would be expected to give better results than IC, but the CA (calculate alone) approach is probably the best method if no spatial output is required. Finally, a methodology was ...

CITE THIS VERSION

Chapter 6

The Consequences of Interpolating or Calculating First on the Simulation of Pesticide Leaching at the Regional Scale

The previous chapter illustrated the differences induced by the choice of interpolating or calculating first in a simple, synthetic case study having one input variable. This chapter explores the same issues in a real case study, in which other factors such as the spatial structure of model inputs may also affect the different modelling approaches.

From this chapter onward, pesticide leaching assessments will be performed for atrazine leaching potential from agricultural sources only. This seems contradictory with respect to the findings of chapter 4, which underlined the non-agricultural origin of atrazine contamination in the Brusselian aquifer. However, there is currently no model equivalent to GeoPEARL for the assessment of pesticide leaching from non-agricultural sources, and developing such tools was not addressed in this thesis. Nevertheless, the immediate consequence of the contradiction noted here is that groundwater monitoring data could not be used to validate atrazine leaching simulations from agricultural land use. The work presented in the following chapters is still relevant because it deals with modelling issues and methods applicable to any other case studies.

6.1 Outline

We analyse different approaches to process soil information when simulating pesticide leaching to groundwater at the regional scale. The first approach, *calculate alone* (CA), consists of the model application on point data followed by the aggregation of the results to the regional scale. Two further approaches are used to generate spatial output and differ by interpolating after or before the model run on point support (*calculate first, interpolate later*; CI vs. *interpolate first, calculate later*; IC). The three approaches are tested with both a linear (modified Attenuation Factor, AF; Rao et al., 1985) and a non-linear (GeoPEARL; Tiktak et al., 2002, 2003) leaching model. The non-linearity of GeoPEARL appears to produce differences between CI and IC that do not occur in the linear model. The results also suggest that the relevance of either CI or IC is dependent on the available input information. Finally, different ways to estimate the prediction precision of the three approaches are discussed[1].

6.2 Introduction

A recurrent issue in the modelling of soil processes is the discrepancy of the spatial support for which a process model was conceived and the support needed for practical soil and water management (Refsgaard and Butts, 1999; Vanclooster et al., 2004a). Basic knowledge of soil processes is generally gained through experiments on soil profiles or pedons. For this reason, soil process models are usually developed at such scales, which will be referred to as the *point support*. Conversely, the geographical area over which models are used has gradually increased (Addiscott and Tuck, 1996), and current needs e.g. for environmental management, have extended the range of model applications across several spatial scales (catchment, regional, global).

Soil process models developed for the point support cannot be assumed to remain valid when used at block supports of tens or hundreds of metres, which is often the size of numerical grids in a spatially distributed

[1]This chapter is based on an article by Leterme B., Vanclooster M., van der Linden A.M.A., Tiktak A. and Rounsevell M.D.A. (20006); published in *Geoderma* doi:10.1016/j.geoderma.2006.09.004.

model. A possible way to overcome this problem is the upscaling of *point models* to broader scales. Refsgaard and Butts (1999) classified upscaling approaches into three groups: (i) local scale equations are assumed valid at the larger scale without any change, (ii) local scale equations are extended in a theoretical framework to account for the spatial variability of smaller scale parameter variability within the block, and (iii) new equations are developed particularly for the broader scale. These procedures all assume that the model is running on the larger block support. Beven (1995) and Heuvelink and Pebesma (1999) argued that the first option is not viable if model equations were established at the point support, and some model parameters were calibrated at the same support. Moreover, due to the variability within the larger block units, any non-linear relationship describing small scale processes will be unreliable when directly applied to the larger scale (Rastetter et al., 1992).

Another means of moving from point to block support is by spatial aggregation of point simulations (Heuvelink and Pebesma, 1999). Three different approaches are possible before the aggregation of model outputs (Addiscott and Tuck, 1996; Heuvelink and Pebesma, 1999). (i) Model runs are performed on all available point inputs followed by interpolation of the model outputs. (ii) Model input parameters are first interpolated, and subsequently the model is run for all points. (iii) A process model is run on point support within a block without interpolating input or point simulated output. Henceforth CI will denote the first approach (*calculate first, interpolate later*), IC the second (*interpolate first, calculate later*) and CA the last approach (*calculate alone*). However, the interpolation-based approaches (CI and IC) are conditionally biased compared to the CA method and will therefore present less variability in their outputs. The CI and IC approaches are appropriate if information about the spatial variability of the output is needed, while CA can be used for aggregating the results in a statistical sense without displaying them spatially.

Addiscott and Bailey (1990) found considerable discrepancy between the CI and IC procedures using a solute leaching model. Stein et al. (1991) tested the same two approaches against field observations to simulate moisture deficits. They found that CI procedures consistently performed better (lower mean squared errors) than IC procedures. Sinowski et al. (1997) compared CI and IC approaches for the regionalization of soil water retention curves.

Considering the effect of land use on input parameters (e.g. organic carbon), they adopted a residual variogram method which lead to better results with the IC procedure. In a field-scale simulation of reactive solute transport, Bosma et al. (1994) showed that the optimal procedure depended on the output of interest. For the calculation of the average solute breakthrough, a more efficient IC procedure could be used in combination with a smaller data set. If the concentrations at specific locations in the field were required, a CI procedure performed better than an IC procedure with smaller data sets. In the calculation of methane emissions, Van Bodegom et al. (2002b) compared the IC approach with process-based simulations based solely on soil profiles. Computing output cumulative density functions, they found that the mean CH_4 emission was hardly influenced at all. However, the spatial heterogeneity in emissions was decreased significantly with the IC approach, relative to point outputs on soil profiles. They did not try to interpolate the latter results (CI).

Heuvelink and Pebesma (1999) suggested that interpolation should take place before the model is run (i.e. the IC approach) because this could enable a more efficient use of the spatial distribution characteristics of individual inputs. They illustrated this point with a linear pedotransfer function, but it should be noted that their IC application benefited from cross-correlation between the two interpolated variables.

Building on the above mentioned studies, aggregation of point information to block support is analysed in the present study for regional scale pesticide leaching. In the context of groundwater management, this application is relevant to assess groundwater vulnerability to pesticide contamination. The first objective of the study is to investigate how the correlation structure and the spatial information about input parameters can influence the results of the CI or IC approach.

A second objective is to find the influence of model non-linearity on any differences between the CI, IC and CA approaches. The proposed methodologies will therefore be tested with both a linear and a non-linear pesticide leaching models. For the linear model, use is made of a linearised version of the Attenuation Factor (AF; Rao et al., 1985). For the non-linear model, the GeoPEARL model (Tiktak et al., 2002, 2003) is used. The latter is a spatial version of the PEARL model which is a reference model in pesticide registration.

Attention will be given to the impact of the selected procedure on the simulated spatial distribution (CI and IC cases) or statistical distribution (CA case) of leaching, in particular calculated leaching percentiles. It is important to consider leaching percentiles, since these are often considered as decision variables in operational risk assessment (Boesten et al., 1999; FOCUS, 2000; van der Linden et al., 2004). Hence, an important objective of the present study was to investigate the possible consequences of the adoption of the CA, CI or IC approaches on the derivation of such statistical indicators.

6.3 Material and methods

The study was undertaken in the Walloon region part of the Dyle catchment (cf. description in chapter 3).

The different models (AF linearised and GeoPEARL) and approaches (CA, CI and IC) were compared for the simulation of atrazine (2-chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine) leaching. In this case, the objective of the modelling is to obtain a spatial image of pesticide leaching (as influenced by the spatial variability in soil properties), and not only the amount of leaching aggregated to the catchment scale.

6.3.1 Soil properties

Data on soil properties were extracted from the Aardewerk soil profile database (Van Orshoven and Vandenbroucke, 1993), and a 1/500,000 soil association map (Maréchal and Tavernier, 1974). The Aardewerk database consists of more than 10,000 detailed soil profile descriptions (i.e. texture, organic matter, pH, etc.) for the different soil horizons for Belgium. The Aardewerk points are not evenly distributed, but 393 profiles (not counting the outlier described in section 6.3.2) were available within the arable part of the study area (Figure 6.1). A buffer zone of 4 km around the study area was included because neighbouring soil profiles could provide valuable information. The representativity of the Aardewerk profiles was assessed by comparing the profile types with the soil map. The results (not shown) indicated that the soil profiles accurately represented the variability of soil properties in the study area. Since AF and GeoPEARL were developed for the assessment of pesticide leaching from agricultural sources, only soil profiles with arable land use were considered. For the soil input parameters not available in Aardewerk, pedotransfer functions (PTFs) were used. The same PTFs were chosen as used in the parameterisation of the GeoPEARL model in order to remain consistent. Soil dry bulk density was calculated with the PTF of Bollen et al. (1995) and the PTFs of Wösten et al. (2001) were used to derive the parameters of the water retention equations (van Genuchten, 1980).

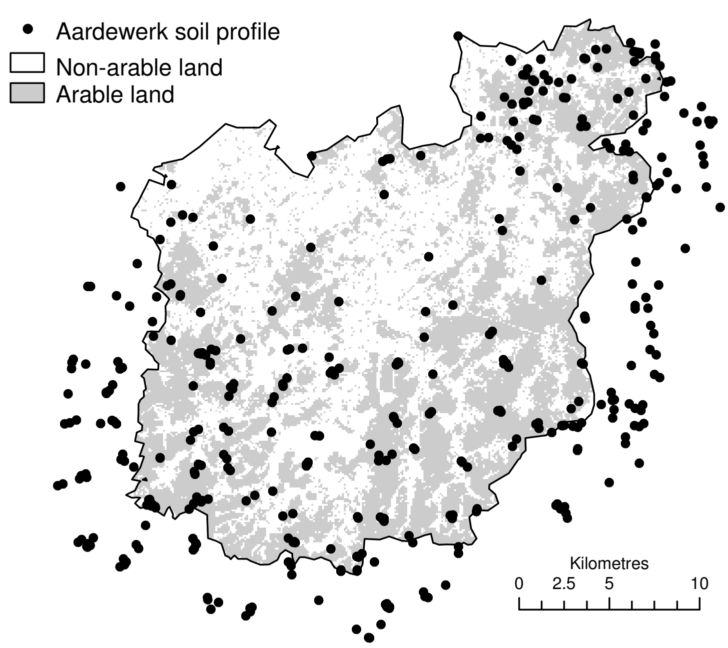

Figure 6.1: Land use and spatial distribution of the soil profiles in the study area (including a buffer zone of 4 km). Only the soil profiles located on arable land were selected in the Aardewerk database.

In practice, the texture fractions and organic matter content were the only properties requiring interpolation in the IC approach because PTFs were used to derive all other parameters needed for the AF_T and GeoPEARL schematisation. The organic matter content and soil water content at field capacity of the top horizon were interpolated using ordinary kriging. No correlation was assumed between organic matter content and texture, as the absolute values of the coefficients of correlation were near zero (< 0.05) for the three texture fractions. For the interpolation of texture fractions, the Bayesian maximum entropy (BME) approach was chosen, which allows the inclusion of hard (accurate) and soft (vague) data in a spatial estimation context (Christakos, 1990, 2000). A variant of the regular BME algorithm using a Monte Carlo procedure, called BME/MC (D'Or and Bogaert, 2001; Bogaert and D'Or, 2002), was used because it takes into account the fundamental constraints on the textural fractions (they sum to one and belong to the $[0, 1]$ interval). In this study, hard data were the texture fractions of Aardewerk profiles, and soft data for all the interpolation points consisted of probabilities of texture fractions derived from the texture classes of the 1/500,000 soil association map.

$\mathrm{AF_T}$ simulations were limited to the top horizon, and the output of GeoPEARL was assessed at 25 cm depth (bottom of the top horizon). The choice of limiting the simulations to the first soil horizon was made because it was not possible to interpolate organic matter and texture properties for the deeper soil horizons. The IC approach would then have needed to use average profiles at depth, and this would decrease the output variability compared to the CI approach on the original complete profiles (results not shown here). Furthemore, it was considered that working on the top horizon only could be justified because, for atrazine, most of the degradation occurs in this layer.

6.3.2 Pesticide leaching index based on the linearised Attenuation Factor

The Attenuation Factor (AF) of Rao et al. (1985) is probably one the most widely used pesticide screening tools. It has been applied both for pesticide screening purposes (e.g. Kleveno et al., 1992; Li et al., 1998) and to assess groundwater vulnerability in a spatial sense (e.g. Loague et al., 1996; Diaz-Diaz and Loague, 2000). The definition of AF is:

$$\mathrm{AF} = \exp\left(\frac{-\ln(2) \cdot d \cdot \mathrm{RF} \cdot \theta_{FC}}{q \cdot DT_{50}}\right) \tag{6.1}$$

where d is the distance to the water table or another reference depth

(L), RF is the Retardation Factor (-), θ_{FC} is the soil water content at field capacity (L^3 L^{-3}), q is the mean annual groundwater recharge (L T^{-1}), and DT_{50} is the pesticide half-life (T).

For a non-volatile pesticide (i.e. the vapour phase is not included), the Retardation Factor is defined as:

$$\mathrm{RF} = 1 + \frac{\rho_b \cdot f_{OC} \cdot K_{OC}}{\theta_{FC}} \tag{6.2}$$

where ρ_b is the soil dry bulk density (M L^{-3}), f_{OC} is the soil organic carbon content (M M^{-1}), and K_{OC} is the pesticide sorption coefficient (L^3 M^{-1}). RF represents the retardation of a pesticide leaching through the soil as a result of partitioning between the soil and liquid phases. Values higher than 1 indicate a lower mobility of the compound.

To obtain a linear model, the first step was the application of a logarithm transformation:

$$\begin{aligned} \ln(\mathrm{AF}) / (-\ln(2)) &= \frac{d \cdot \mathrm{RF} \cdot \theta_{FC}}{q \cdot DT_{50}} \\ &= d \cdot \frac{\theta_{FC} + \rho_b \cdot f_{OC} \cdot K_{OC}}{q \cdot DT_{50}} \end{aligned} \tag{6.3}$$

In this study, θ_{FC}, ρ_b and f_{OC} were spatially variable, while other inputs in Eq. (6.3) were held constant. However, non-linearity is still present in Eq. (6.3) in the factor $\rho_b \cdot f_{OC}$, since ρ_b was calculated using a pedotransfer function in f_{OC}. Therefore, a linear regression was fit to this factor to make it dependent only on f_{OC} (Figure 6.2). The dashed line in Figure 6.2 shows the regression with all data (394 soil profiles). Even though the fit was already good ($R^2 = 0.87$), it was believed that the regression could be improved by the removal of the outlier located at $f_{OC} = 0.16$. This increased the R^2 to 0.97. The removal of this outlier is justifiable. The main argument is that a f_{OC} of 0.16 is very unlikely for an arable soil profile in the sandy loam or loamy soils of the study area. Using the same database as in the present study (cf. section 6.3.1), van Wesemael et al. (2004) compiled carbon stocks and confidence intervals for arable land use in different soil associations. Converting their results to f_{OC} values, the

95% confidence interval on the mean for the soil association corresponding to the outlier was $f_{OC} = 0.0194 \pm 0.0007$. Thus, it was strongly suspected that the outlier was either an error in the database, or a specific profile (e.g. sampling occured shortly after land conversion from grassland).

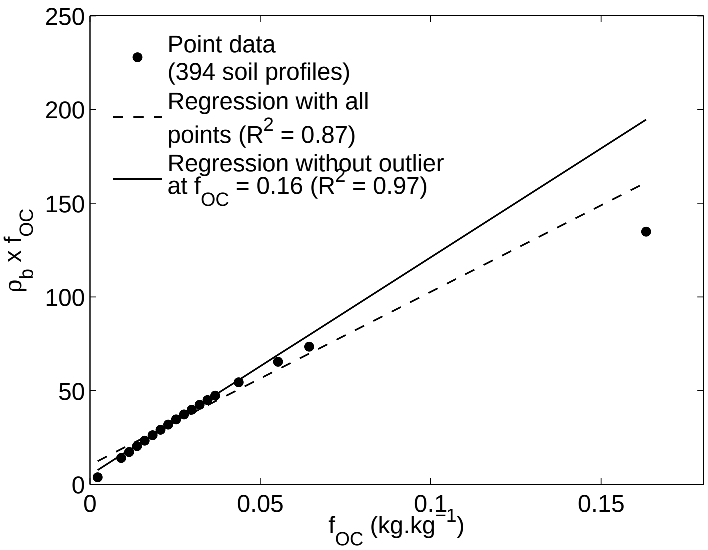

Figure 6.2: Linear regression with $[\rho_b \times f_{OC}]$ as the dependent variable and f_{OC} as the independent variable. The regression fit is shown with all data (dashed line; $N = 394$ and $\mathrm{R}^2 = 0.87$) and without the outlier plotted at $f_{OC} = 0.16$ (solid line; $N = 393$ and $\mathrm{R}^2 = 0.97$).

Using the estimates of the regression parameters, Eq. (6.3) is further transformed to obtain a new linear form of the AF index, $\mathrm{AF_T}$:

$$\mathrm{AF_T} = d \cdot \frac{\theta_{FC} + (\hat{\beta}_0 + \hat{\beta}_1 \cdot f_{OC}) \cdot K_{OC}}{q \cdot DT_{50}} \tag{6.4}$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are estimates of the regression parameters.

$\mathrm{AF_T}$ is then rescaled between 0 and 1 (giving $\mathrm{AF_{T_{0-1}}}$) using the minimum and maximum values among the pooled outputs of the two approaches (i.e. relative comparison is possible between CI and IC). A pesticide leaching index is then calculated as:

$$\text{Leaching index} = 1 - \text{AF}_{\text{T}_{0-1}} \tag{6.5}$$

This last transformation allows easier comparison with the simulations of GeoPEARL (i.e. a higher score means higher leaching). The pesticide leaching model described above is further referred to as the AF_T model.

6.3.3 Pesticide leaching simulated with GeoPEARL

The model GeoPEARL (Tiktak et al., 2002, 2003) was chosen to perform the simulations of atrazine leaching. GeoPEARL resulted from the coupling of the PEARL model (Tiktak et al., 2000) with spatial input files that can be derived from a standard Geographical Information System. PEARL is a one-dimensional, dynamic, multi-layered model of the fate of pesticides and relevant transformation products in the soil-plant system. The model is linked to the Soil Water Atmosphere Plant (SWAP; Van Dam, 2000) model for the hydrology.

Annual (spring) applications of atrazine were simulated for silage maize cropping. Atrazine properties were taken as constant. The simulation period was fixed from 1980 to 2002, including a buffer of 6 initialisation years. Annual average concentrations of atrazine at 25 cm depth were extracted from the simulation results. This depth corresponds to the bottom of the topsoil horizon. Groundwater vulnerability was then assessed by taking the median of the annual average concentrations (total of 17 simulation years). Finally, these median values were rescaled to between 0 and 1, using the minimum and maximum values of both the CI and IC approaches. This produced a pesticide leaching indicator allowing relative comparisons.

In this study, only soil properties were considered to be spatially variable, as test simulations showed the variability of climatic factors to be less important (results not shown). This is intuitive because at the scale of the Dyle catchment area, spatial variability in the weather is small. For larger areas, climatic conditions would be much more important (e.g. Bleecker et al., 1995).

6.3.4 Calculate alone, and calculate or interpolate first: CA, CI and IC approaches

The CA approach involved no interpolation at any stage. It consisted of running the model (AF_T or GeoPEARL) on the 393 Aardewerk soil profiles (Figure 6.1). The output variable (AF_T and median of annual average concentrations, respectively) was then derived from this point support. Using ancillary information is a possible option to map the results of the CA approach. For example, a soil map may be used to delineate polygons as mapping units, over which the results are obtained by a weighting procedure of the point outputs according to their soil properties. However, this particular approach will not be adopted, because the soil association map used in this study has a classification scheme that is too coarse—the three main soil associations covering over 95% of the study area (i.e. a lot of the soil variability displayed by the soil profiles would be lost).

The CI approach further involved the interpolation of the output variable. A semivariogram model was fitted to this variable to allow interpolation (using ordinary kriging) to a 100×100 m grid.

The IC approach began with the interpolation of organic matter content (using ordinary kriging) and the soil water content at field capacity (for AF_T; using ordinary kriging) or the texture fractions (for GeoPEARL; using BME/MC). The second step then consisted of running the model (AF_T or GeoPEARL) on point support (26602 points on a 100×100 m grid).

Ordinary kriging is a classical type of kriging where the spatial variation is spatially homogeneous and the mean function is not known or difficult to estimate (Christakos et al., 2002). It was considered appropriate for this study, with the soil properties showing virtually no deterministic variation in the study area (only arable land use). With a linear model and simple or ordinary kriging for the interpolation, the CI and IC approaches would yield the same result because kriging is a linear operator (Heuvelink and Pebesma, 1999). However, results can differ between CI and IC if co-kriging (or any other techniques involving ancillary information) is used for the interpolation of input variables. In the case of non-linear models, the two approaches are strongly expected to produce different outputs. A process-based model, such as GeoPEARL, combines non-linear processes and interactions. A discrepancy can therefore be expected between the average output value and the output obtained with interpolated input parameters. For complex models, it can be quite difficult to anticipate how non-linearity will affect the differences between CI and IC. There may be differing degrees of non-linearity (Addiscott and Tuck, 2001). With a simple example, Addiscott and Tuck (1996) showed that the semivariogram of an input soil property used as a model parameter can influence the output from the model. They suggested that this influence could be expected for any non-linear model.

After the application of CI or IC, Heuvelink and Pebesma (1999) suggested to proceed further with an aggregation step, i.e. the aggregation of point support information to block support using simple averages. The whole procedure of kriging followed by aggregation is known as 'block kriging' (Heuvelink and Pebesma, 1999). The aggregation step cannot be applied earlier in the sequence because of model non-linearity. Due to variability among the components being aggregated, any non-linear model would be unreliable when directly applied to the aggregate (Rastetter et al., 1992). In the present study, the main objective is to compare the CI and IC approaches. The aggregation step was performed, but only to evaluate the persistence of the results under spatial aggregation. Another possibility is to consider the entire catchment as the block support.

Although this study presents a practical application of the upscaling procedures presented above, a few theoretical considerations need to be made here.

First, the CI approach would be expected to give better results than the IC approach, especially if the uncertainty about the interpolated input values is not processed in the model run. This could have adverse effects when, for example, interpolation is likely to yield poor results because of weak spatial correlation of input variables (short range or high nugget effect). Furthermore, the continuous map of interpolated values should not be considered to contain more information than a finite set of input values. Interpolation procedures such as kriging do not add information but instead affect the way information is distributed over space.

Secondly, model input values that are obtained from kriging do not have the meaning of values but are conditional expectations. Models are supposed to process values, but when using IC they are fed with conditional expectations, which by definition have much less variability than raw values, so one would expect in turn less variability in the model outputs.

Finally, for management purposes, CI and IC approaches should be discarded if no spatial output is required, as they would only add uncertainties difficult to correctly account for. For several applications that aim at deriving global estimates, mapping it is thus baseless.

6.3.5 Comparison of the results

Two main tools were available to examine the differences between the four different vulnerability assessments (two models and CI/IC approaches). One was the comparison of the output maps, and the other was the comparison of the cumulative density functions (CDFs) computed at the catchment scale.

The comparison of output maps was performed using the statistical measures of Pontius et al. (2005). This method compares two maps that show (different) patterns of the same real variable. The method was initially developed to compare a simulation against observed values, but it can be applied to the present case by assuming that, for example, the IC approach is the 'reference' map. The technique of Pontius et al. (2005) budgets the agreement and disagreement between the maps in terms of the components of quantity (i.e. overall average) and location (i.e. spatial arrangement) of the variable. These budgets (see Eq. (5.5) to (5.10) in chapter 5) were computed using both the root mean square error (RMSE) and the mean absolute error (MAE).

A detailed description of the different components of these equations are given in chapter 5 (section 5.3).

A possible drawback of these budget equations is that the component 'agreement due to location' is not the same if we switch the maps (i.e. which is the 'comparison' map giving the $\overline{Y}$ value, and which is the 'reference' map ?). Choosing the reference map is not obvious; both maps can serve as a reference. The original method compares predicted values with observed values and in this case the problem does not exist (Pontius et al., 2005). Nevertheless, this had no implications for the interpretation of the results because the maps were compared relatively to one another. The general conclusions deriving from the map comparison were therefore not affected by the choice of the 'reference' map (IC approach).

The differences in shapes of the CDFs were tested by an adaptation of the Kolmogorov-Smirnov (KS) test. This test assumes independence, which is not true for the spatially correlated data used in this study. The CDFs comparison was therefore made using KS in a Monte Carlo permutation test (Manly, 1997). In this methodology, the null hypothesis (H_0) is that the two distributions are identical; i.e. they are two samples from the same population. The distribution of the KS statistic under H_0 is obtained by deriving permutations of the grouped observations in all possible ways ($N =$ 9999 here) and with equal probabilities. This distribution is then used to calculate the significance of the test as:

$$p_{value} = \frac{1 + \#(\mathrm{KS}_i > \mathrm{KS}_0)}{1 + N} \tag{6.6}$$

where KS_i is the KS statistic of the i^{th} permutation and KS_0 is the value of the KS statistic for the original two samples. This statistical analysis of the CDFs is not spatially explicit and the test is liberal in the sense that it tends to reject the null hypothesis of equality of CDFs too often (Van Bodegom et al., 2002b).

Table 6.1 summarizes the available outputs for the three methodologies examined in this study (CA, CI and IC).

Table 6.1: Available outputs for the three approaches CA, CI and IC.

$\mathrm{AF_T}$ / GeoPEARL	Map	CDF
CA		✓
CI	✓	✓
IC	✓	✓

6.4 Results

6.4.1 Maps comparison of CI vs. IC

AF_T model

Figures 6.3(a) and (b) present for the AF_T model the maps of the CI results and of the difference between IC and CI, respectively. The values of the indicator were rescaled to between 0 and 1 to allow easier comparison (the minimum and maximum values of the different approaches before normalization are shown in Table 6.2). The amplitude of the differences in Figure 6.3(b) is very low. This was expected because the algorithm of ordinary kriging is a linear estimator, and so both approaches (CI or IC) only involved linear operators (linear model and kriging) for which the order of their application is not important. This situation is different from studies where cross-covariance between input variables is considered for the IC approach, but is not relevant to the CI method.

Figure 6.4 shows the results of the map comparison using the Pontius et al. (2005) budget equations (cf. Eq. (5.5) to (5.10)). It can be seen that the two maps are not exactly the same, because there is a small disagreement due to quantity in both the Root Mean Square Error (RMSE) and Mean Absolute Error (MAE) calculations, and a small disagreement due to location in the RMSE budget. However, the agreement due to location is clearly dominant, thus implying that both approaches would deliver nearly identical outputs in a management context. The slight initial increase of agreement due to location in the MAE calculation (Figure 6.4(b)) is probably an artefact of the aggregation step due to the non-regular coverage of arable land. The minor differences underlined by the components of disagreement can be attributed to differences in the semivariogram fitting between CI and IC. Since the exact models are not known, some differences can result from the estimation of semivariogram parameters (e.g. choice of the model type, distance classes, etc.), although these parameters were assessed as objectively as possible. Table 6.3 displays the parameters obtained for the different approaches.

The magnitude of the nugget effect is comparable between IC and CI. Organic matter content, interpolated using ordinary kriging, was characterised

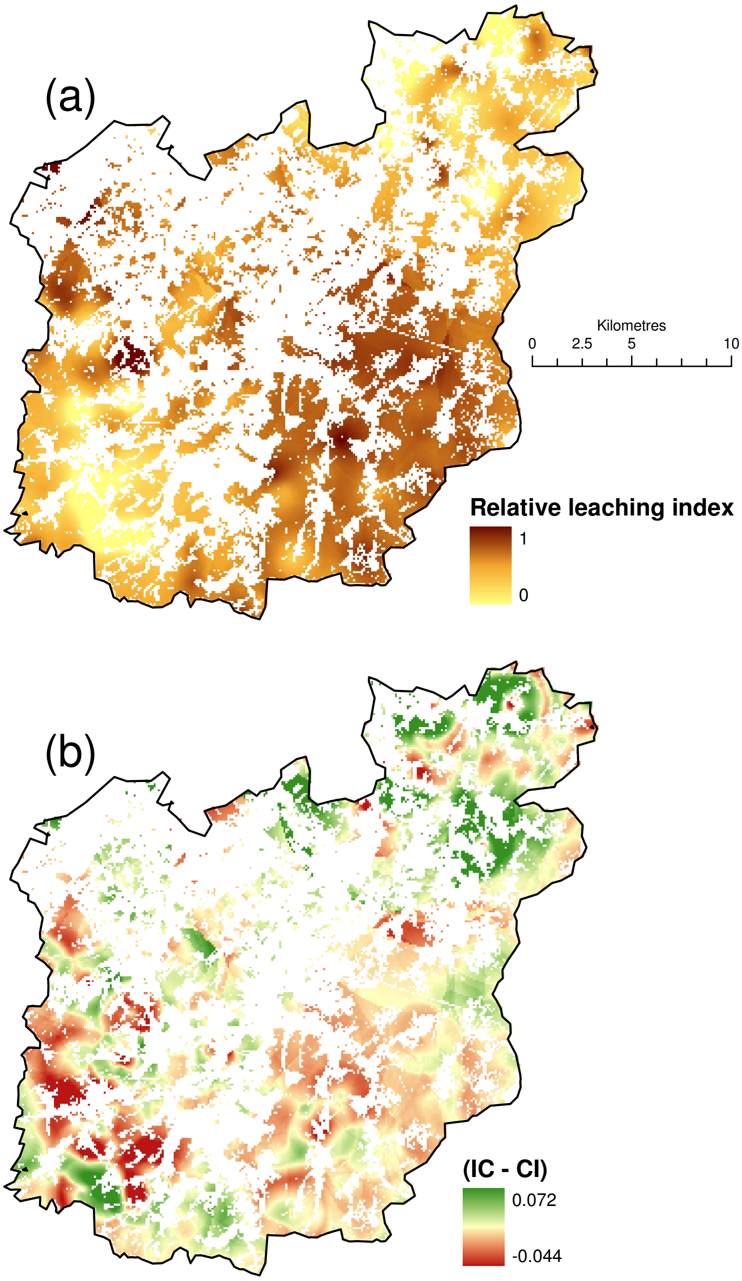

Figure 6.3: Maps showing the relative leaching index calculated by the linear AF_T model. (a) CI approach and (b) difference between IC and CI. White areas are non-arable land.

Table 6.2: Minimal and maximal values before normalization of the outputs of the AF_T and GeoPEARL models, for the three approaches CA, CI and IC. The output of the AF_T model is calculated by Eq. 6.4, while the output of GeoPEARL is the median of the annual average concentrations.

	AF_T (-)		GeoPEARL (μg/L)	
	Min.	Max.	Min.	Max.
CA	2.94	4.46	0.15	40.40
CI	3.32	4.15	6.67	18.51
IC	3.31	4.16	4.41	19.40

Table 6.3: Parameters of the semivariogram models used in the IC (interpolation of organic matter content, soil water content at field capacity and texture) and CI approaches (interpolation of the AF_T and GeoPEARL outputs).

	Semivariogram parameters		
Variable	Model type (Nugget + ...)[a]	Nugget effect (% of total variance)	Actual range (m)
f_{OC}	Exponential	41	1775
θ_{FC}	Spherical	40	1685
Texture	LMC[b] - Spherical	48 to 62	2800
AF_T	Spherical	48	1855
GeoPEARL	Spherical	53	9860

[a] All the semivariograms had a nugget effect.

[b] Linear Model of Coregionalisation (LMC) based on the covariance matrices for the three textural fractions - sand, silt and clay - and for which the range had to be fixed by the user.

by a nugget effect representing 41% of the total variance and a practical range of 5325 m. The practical range refers to the distance where the semivariogram model meets the variance. For exponential models, this is defined as 95% of the variance, and the actual range is one third of the practical range (Journel and Huijbregts, 1978). Thus the value of (5325/3 =) 1775 m should be considered as the correlation range of organic matter content (Table 6.3). For the spherical model, the actual range is equal to the practical range. The output variable of the AF_T model had a correlation range of 1855 m, which can be regarded as a direct influence of the spatial structure of organic matter and soil water content at field capacity, both being of the same order of magnitude.

GeoPEARL model

Figures 6.5(a) and (b) present for the non-linear GeoPEARL model the maps of the CI results and of the difference between IC and CI, respectively. The minimum and maximum values of the different approaches before normalization are shown in Table 6.2. It is important to note here that the spatial patterns simulated by GeoPEARL are substance dependent. This analysis was limited to atrazine, but the results for a mobile substance such as bentazone may be different. Visual comparison suggests that the IC map reflects the soil map used in the interpolation of the textural fractions in some locations. In Figure 6.5(b) typical soil map boundaries can be observed in the form of abrupt changes, notably in the Western part of the study area. There, a higher organic matter content was reflected by the low values of the pesticide leaching index, except in the IC approach where the soil map located more sandy soils in some places (the darker zones in Figure 6.5(b)). More generally, the CI approach displays smooth spatial variation (Figure 6.5(a)).

The non-linearity of GeoPEARL appears to strongly affect the correlation range of its output variable compared to the ranges of input parameters (Table 6.3). The output variable of GeoPEARL has a range of 9860 m, while the ranges of inputs are respectively 1775 and 2800 m (actual ranges of organic matter content and texture fractions). The range of texture fractions was fixed by eye, while the nugget effect varied between 48 and 62% for the six (cross-)semivariograms of the three textural fractions. This differ-

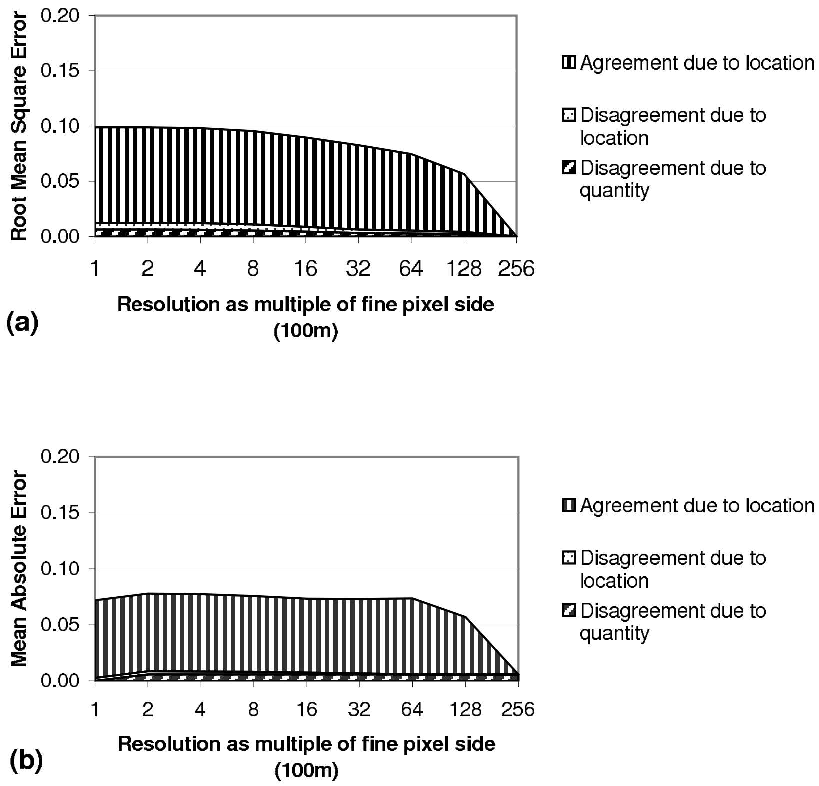

Figure 6.4: Multiple resolution budget of components of information based on (a) Root Mean Square Error and (b) Mean Absolute Error. Eq. 5.5 to 5.10 are used to compare the maps of the CI and IC approaches for the AF_T model, as a function of the level of spatial aggregation.

ence in semivariogram ranges can be noticed in Figure 6.5. The leaching index displays smooth spatial variations in Figure 6.5(a), while variability within shorter distances can be distinguished in Figure 6.5(b), notably in the South-Eastern part of the study area.

The budget equations allowed quantification of the (dis)similarity between the CI and IC maps, as shown in Figure 6.6. The disagreement due to quantity (independent of block support resolution) remains constant using either Root Mean Square Error (RMSE) or Mean Absolute Error (MAE) calculations. This error in quantity indicates the differences in averages between the two maps. This time a significant disagreement due to location is found, especially in the RMSE budget equations (Figure 6.6(a)). This indicates that the spatial pattern was affected by the choice of the CI or IC approach. However, the component of agreement due to location is superior to the disagreement due to location at almost all resolutions. The agreement due to location means that the spatial pattern of the CI map is more similar to the IC map than to a uniform map with an average CI value. Thus, independently of the CI or IC approach, the spatialisation of pesticide leaching using GeoPEARL reflected the influence of the variables known to play a role in the processes involved (organic matter content, texture, etc.).

The disagreement due to location appears to be caused primarily by the ancillary information (soil map) introduced into the IC approach. Figure 6.6 shows that the disagreement due to location regularly decreases as resolution becomes coarser, while the agreement due to location remains constant until a resolution of $(16 \times 100 =)$ 1600 m. This can be explained by the declining influence of the soil map on the spatial pattern as the aggregation becomes coarser because the soil association map only has an effect on the IC simulations in a small part of the study area (Figure 6.5).

The effect of the non-linearity of GeoPEARL is discernible in two ways. The first is the disagreement due to quantity, which is further detailed in section 6.4.2. The second is the semivariogram range of the CI approach (9860 m), which is significantly higher than the ranges of the inputs used in the IC approach (1775 and 2800 m for organic matter content and texture). Interaction of model non-linearity with the spatial distribution of inputs significantly increases the semivariogram range in the CI approach, thus enhancing the map smoothness between the interpolation points (Figure 6.4(a)).

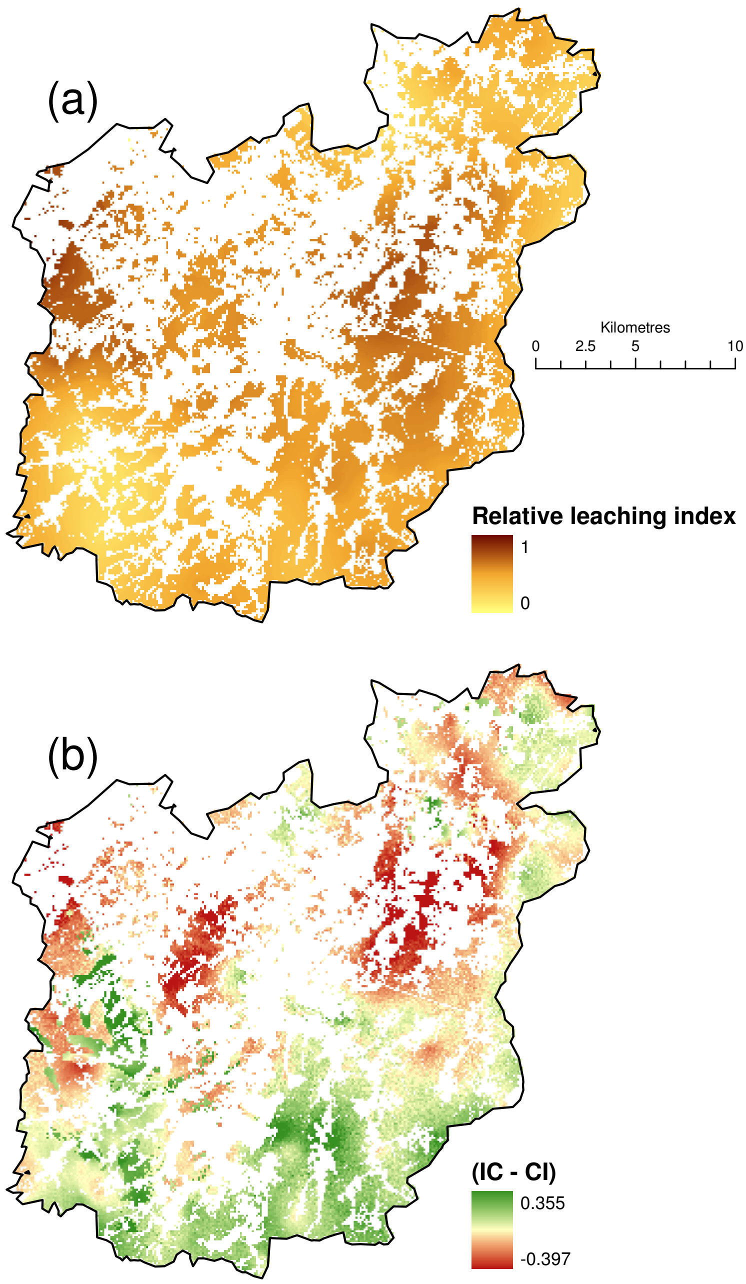

Figure 6.5: Maps showing the relative leaching index calculated by the non-linear GeoPEARL model. (a) CI approach and (b) difference between IC and CI. White areas are non-arable land.

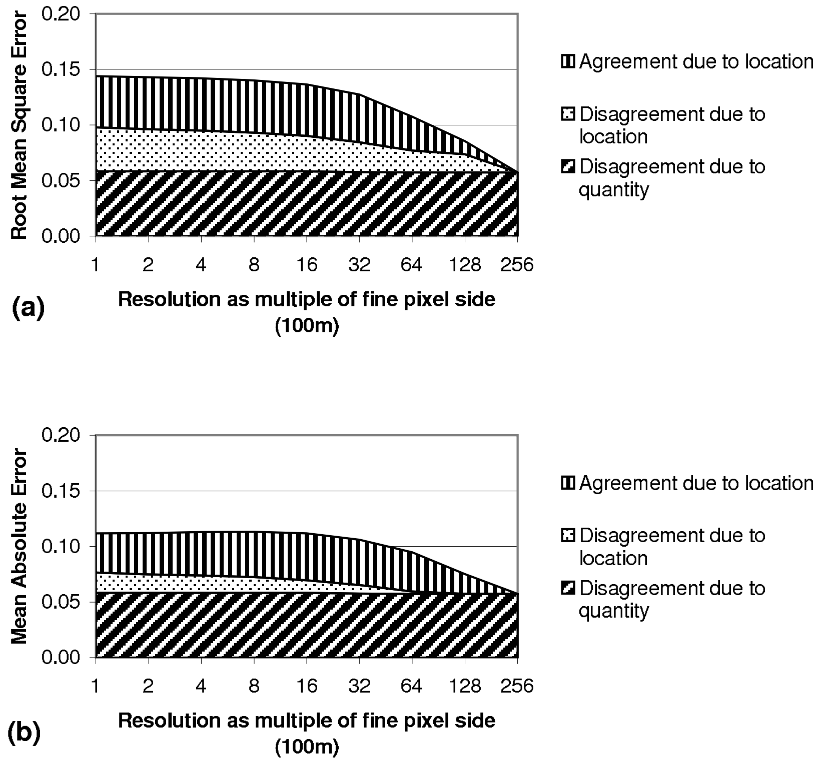

Figure 6.6: Multiple resolution budget of components of information based on (a) Root Mean Square Error and (b) Mean Absolute Error. Eq. 5.5 to 5.10 are used to compare the maps of the CI and IC approaches for the GeoPEARL model, as a function of the level of spatial aggregation.

6.4.2 CDFs comparison

AF_T model

The results can be examined in a non-spatial way (i.e. assuming that the block support is the whole study area) by plotting the cumulative density functions (CDFs) of each approach. Figure 6.7 presents the CDFs for the AF_T model. In addition to the CI and IC curves (solid and dashed lines respectively), this figure presents the results of the CA method (dash-dotted line).

Comparison of the CDFs with the Monte Carlo permutation test (Eq. (6.6)) showed that all three CDFs are significantly different ($p_v = 0.0001$ for each test CI vs. IC vs. CA). Although they are very close to each other, the CI and IC CDFs are significantly different because of the very high n (= 26602) in the Kolmogorov-Smirnov test. However, these results also confirm that the choice of a given methodology e.g. to determine certain vulnerability percentiles is an important factor in the procedure of pesticide leaching assessment, especially in the range of extreme percentiles.

As expected, it can be seen that the greatest differences occurred between CA simulations compared to the CI and IC approaches. The bias due to the interpolation step in the CI and IC results can be observed in the reduction of variability as one passes from point support (CA) to interpolated results, because kriging intrinsically tends to smooth out extreme values.

This has important implications for management purposes. In this particular situation, the assessment of pesticide leaching at the catchment scale is strongly dependent on the decision to choose a mapping approach or not (CI or IC vs. CA). Moreover, percentile calculations for, for example, the screening of new products would be influenced by the chosen approach.

The permutation test was also performed on the aggregated maps. For AF_T, CDFs of CI and IC were no longer statistically different from an aggregation level of 8 onwards (i.e. 800 × 800 m block output). This means that at resolutions equal to, or finer than, 400 × 400 m, the two approaches yield statistically different results.

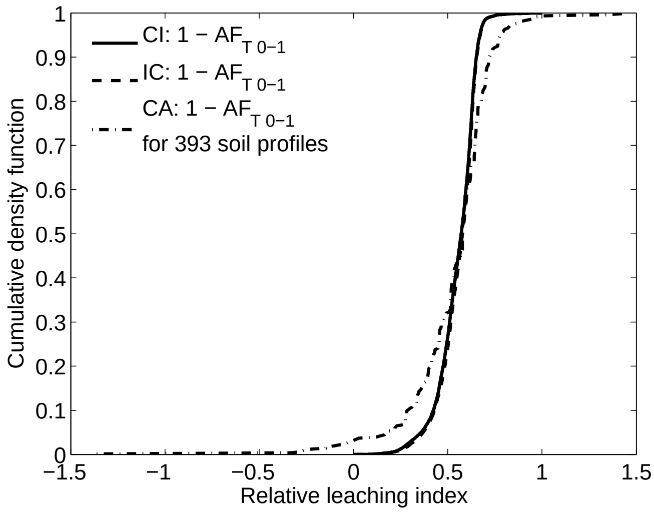

Figure 6.7: Cumulative density function of relative leaching scores calculated with the AF_T method.

GeoPEARL model

Figure 6.8 presents the CDFs for the GeoPEARL model. The main feature of the three CDFs is the much larger spread of the CA distribution. The reasons for this are the same as for the AF_T model. Moreover, the Monte Carlo test showed that all three CDFs are significantly different for the GeoPEARL model ($p_v = 0.0001$ for each test CI vs. IC vs. CA). The horizontal shift between the CI and IC CDFs corresponds to the disagreement due to quantity visible in Figure 6.6. The conclusion for the non-linear GeoPEARL model is that CI gives significantly higher leaching of atrazine than IC, but that the spatial pattern is not significantly affected (cf. agreement due to location in Figure 6.6).

The Monte Carlo test with the aggregated maps yielded different results than for AF_T. The CDFs of CI and IC were not statistically different from an aggregation level of 64 onwards (i.e. 6400 × 6400 m block output, corresponding to the whole study area being covered by 16 blocks). This means that at a coarser resolution than 3200 × 3200 m, the two approaches produced statistically similar results. This can have implications for decision makers, for example when defining the scale at which a pesticide leaching assessment should be undertaken.

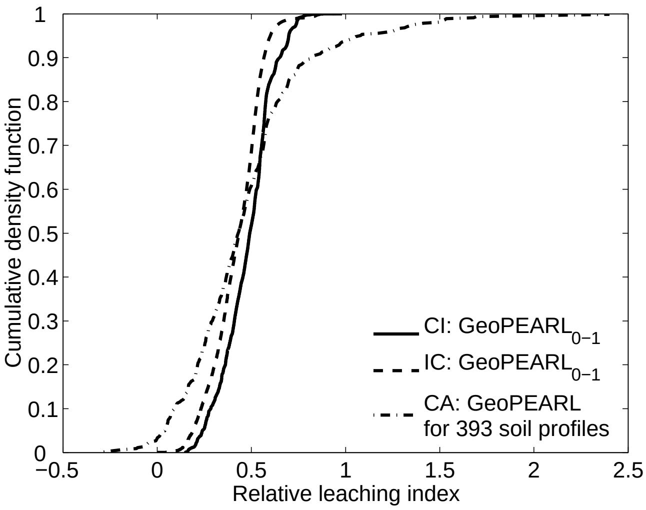

Figure 6.8: Cumulative density function of relative leaching scores calculated with the GeoPEARL model.

6.5 Discussion and conclusions

This study did not consider the effect of uncertainty due to interpolation, but the different ways to tackle this issue are discussed here.

In the CI approach, once the model outputs are calculated on the 393 soil profiles, a simulation-based approach could be adopted instead of kriging. This would lead to the generation of n maps, from which the 80$^{\text{th}}$ percentile in space can be derived repeatedly. A distribution of this target quantity is finally obtained, and decision can be taken for example based on the proportion of simulations above a certain threshold.

In the IC approach, the simulations would generate n maps of the input variables. The model has subsequently to be run on the 26602 point supports for each of the n sets of inputs. Again, a distribution of the target percentile can ultimately be derived from the results.

An important advantage of the CI over the IC approach lies in the computation cost imposed by the uncertainty analyses described above. Applying it to the IC approach would require n simulations ($\times$ the number of input variables) plus 26602 $\times$ n model runs; while CI would only require 393 model runs and n simulations. This argument may become decisive especially if a process-based model like GeoPEARL is used.

However, if some input parameters are cross-correlated, this ancillary information can only be incorporated within the IC approach. This is the reason why Heuvelink and Pebesma (1999) recommended that the IC approach be used instead of CI. However, a lower prediction variance does not necessarily mean that the retained value (the center of the prediction distribution) is better than with the CI approach. A different argument could be that, as interpolation is a tool to 'fill in the missing information', it should be used as a last resort, i.e. via the CI approach. Further investigation is needed, notably via Monte Carlo simulations, to examine whether one of the two approaches could be identified as a better mapping methodology from a theoretical basis.

Bosma et al. (1994) argued that the suitability of CI or IC could depend on the quantity of interest. Similarly, the simulations presented here suggest that the spatial structure of model inputs has a strong influence on the CI and IC approaches. Heuvelink and Pebesma (1999) included the correlation between two variables in the IC approach, whilst the present study used a particular non-linear method (BME/MC) to interpolate texture fractions for the IC approach with GeoPEARL. It is likely that the relevance of either CI or IC could be dependent on the available input information. As Van Bodegom et al. (2002b) concluded, "scaling effects are thus situation dependent and, more specifically depend on data distribution, correlations between data and the relationships between underlying processes that control the entity to be predicted."

For the CA approach, sampling error can be estimated using bootstrap. The sample of 393 model inputs can be re-sampled n times with replacement to assess the uncertainty on the 80^{th} percentile of pesticide leaching. As mentionned earlier, the representativity of the Aardewerk profiles was assessed by comparing the profile types with the soil map. The results (not shown) indicated that the soil profiles accurately represented the variability of soil properties in the study area. If it were not the case, the soil association map can still be used to give different weights to the soil profiles in the bootstrap procedure.

The first objective of this study was to find the influence of the spatial correlation of input parameters in the CI and IC approaches. It was demonstrated that the correlation structure of model input plays a key role in the differences between the CI and IC approaches. For a linear model, the correlation range of input parameters entirely determines the semivariogram range of the output variable in the CI approach. This was not true for GeoPEARL, as the effect of model non-linearity led to a significant increase in the semivariogram range.

More precisely, the second objective of this study was to determine the influence of model non-linearity over the different approaches tested. As expected, the CI and IC approaches gave identical results for the linear model, while two main differences between these approaches occurred in the non-linear case. The first was the increase of the semivariogram range of GeoPEARL outputs in the CI approach, as mentioned above. Secondly, GeoPEARL non-linearity produced the disagreement due to quantity observed between the CI and IC approaches (higher leaching with CI). Thus, model non-linearity can affect both the quantity and spatial pattern of pesticide leaching.

Finally, a typical quantity of interest in legislation is the 80$^{\text{th}}$ percentile of pesticide leaching in space (e.g. FOCUS, 2000). The third objective was to examine the consequences of the adoption of the CA, CI or IC approaches on such indicators.

An issue lies in the fact that interpolation (in CI and IC) is usually designed to predict the unbiased mean value, but not to predict percentiles in an unbiased way. Therefore, in the context of decision making, the CA approach seems the most appropriate if no spatial output is required, considering that CI results will not contain more information than CA when computing global estimates.

The CA approach could even be extended to obtain a spatial output, e.g. by using a soil map as ancillary information to display the results. However, the feasibility and interest of this mapping procedure depends on the balance between the scale of the soil map and the soil variability captured by the point profiles. Using a coarse resolution soil map would lead to the loss of the information within the soil profiles, but too fine a resolution would prevent the allocation of point outputs to all mapping units.

This study insisted on the significant consequences of the adoption of an approach based on interpolation (CI or IC) compared to point-based simulation (CA). This is because the interpolation of environmental variables involves a reduction in the heterogeneity and hence a shift of the target percentiles towards the mean. However, CI and IC are still relevant if they include simulations that take into account the uncertainty due to interpolation.