The consequences of interpolating or calculating first on the simulation of pesticide leaching at the regional scale

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Introduction

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 model. A possible way to overcome this problem is by **spatial aggregation** of point simulations (Heuvelink and Pebesma, 1999).

In this study, three different approaches, denoted **CA**, **CI** and **IC** (see the text beside) were tested with both a **linear** and a **non-linear** pesticide leaching models (modified AF and GeoPEARL).

In the context of **groundwater management**, this application is relevant to assess groundwater vulnerability to pesticide contamination. The **main objective** of the study was to determine how the results of the CA, CI and IC approaches are influenced by **(i)** the **correlation structure** and the **spatial information** about input parameters, and **(ii) model non-linearity**.

Attention was also 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**.

CA, CI, IC

- **CA**: *calculate alone.*

→ Model application on point data (soil profiles) followed by the aggregation of the results to the regional scale

- **CI**: *calculate first, interpolate later.*

→ Model run on point support followed by spatial interpolation of the model outputs

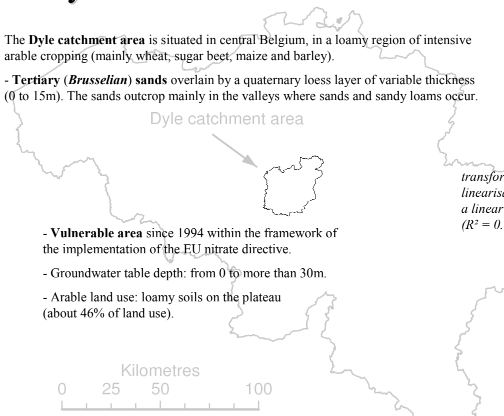
- **IC**: *interpolate first, calculate later.*

→ Interpolation of the model inputs followed by model application

Study area

The **Dyle catchment area** is situated in central Belgium, in a loamy region of intensive arable cropping (mainly wheat, sugar beet, maize and barley).

- **Tertiary (*Brusselian*) sands** overlain by a quaternary loess layer of variable thickness (0 to 15m). The sands outcrop mainly in the valleys where sands and sandy loams occur.



- **Vulnerable area** since 1994 within the framework of the implementation of the EU nitrate directive.

- Groundwater table depth: from 0 to more than 30m.

- Arable land use: loamy soils on the plateau (about 46% of land use).

Two Models

Linear model: modified Attenuation Factor

(AF; Rao et al., 1985)

$$
\begin{cases}
AF = \exp\left(\dfrac{-\ln(2)\cdot d \cdot RF \cdot \theta_{FC}}{q \cdot DT_{50}}\right) \\[2ex]
RF = 1 + \dfrac{\rho_b \cdot f_{OC} \cdot K_{OC}}{\theta_{FC}}
\end{cases}
$$

transformation and linearisation using a linear regression ($R^2 = 0.97$)

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

d is the distance to the reference depth (L), θ_{FC} is the soil water content at field capacity ($L^3\ L^{-3}$), $\hat{\beta}_0$ and $\hat{\beta}_1$ are estimates of the regression parameters, f_{OC} is the soil organic carbon content ($M\ M^{-1}$), K_{OC} is the pesticide sorption coefficient ($L^3\ M^{-1}$), q is the mean annual water recharge ($L\ T^{-1}$) and DT_{50} is the pesticide half-life (T).

θ_{FC} and f_{OC} are **the only variables**. All other parameters are taken as constant.

Non-linear model: GeoPEARL

(Tiktak et al., 2002, 2003)

GIS coupled to a **one-dimensional**, **dynamic**, **multi-layered** model of the fate of pesticides and relevant transformation products in the soil-plant-atmosphere system.

Results

1) Maps comparison of CI *vs.* IC

Visual comparison of the two maps displayed here suggests that the IC map reflects the soil map used in the interpolation of the textural fractions in some locations.

In **Fig. 1b** typical **soil map boundaries** can be observed in the form of abrupt changes. The CI approach displays smooth spatial variation (**Fig. 1a**).

GeoPEARL non-linearity strongly affected the **correlation range** of its output variable compared to the ranges of input parameters (**Table 1**). This was not the case for the linear **AF_T model**.

Budget equations from Pontius et al. (2005) allowed quantification of the (dis)similarity between the CI and IC maps, as shown in Fig. 2.

The **disagreement due to quantity** (independent of block support resolution) indicates the differences in averages between the two maps.

The significant **disagreement due to location** indicates that the spatial pattern was affected by the choice of the CI or IC approach.

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 a pesticide leaching index using GeoPEARL reflected the influence of the variables known to play a role in the processes involved (organic matter content, texture, etc.).

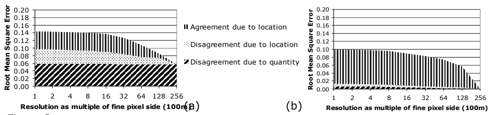


Figure 2:
Multiple resolution budget of components of information based on Root Mean Square Error. Comparison of CI and IC for the (a) GeoPEARL and (b) AF_T models.

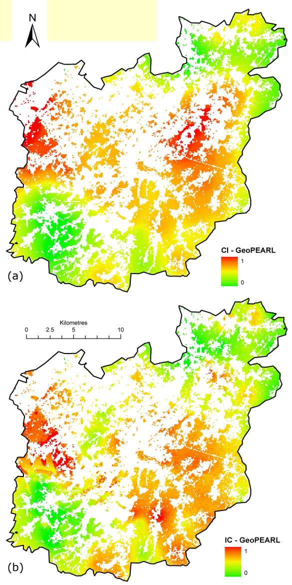


Figure 1:
Maps of the relative leaching index using the non-linear GeoPEARL model and the (a) CI and (b) IC methodology. White areas are non-arable land.

2) Cumulative density functions at the regional scale

Table 1:
Parameters of the semivariogram models used in the IC (interpolation of f_{OC}, θ_{FC} and texture) and CI approaches (interpolation of the AF_T and GeoPEARL outputs).

Variable	Semivariogram parameters		
	Model type (Nugget + …)	Nugget effect (% of total variance)	Range (m)
f_{OC}	Exponential	41	5325
θ_{FC}	Spherical	40	1685
Texture	LMC[a] – Spherical	48 to 62	2800
AF_T	Spherical	48	1855
GeoPEARL	Spherical	53	9860

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

Texture fractions were interpolated using the Bayesian Maximum Entropy/Monte Carlo algorithm (Bogaert and D'Or, 2002), which combines *hard* (soil profiles) and *soft* (soil map) data.

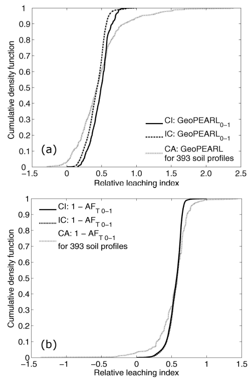


Figure 3:
Cumulative density functions of relative leaching scores calculated with the (a) GeoPEARL and (b) AF_T models.

Conclusion

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**.

This study did not consider **uncertainty due to interpolation**. The kriging prediction is not a deterministic value, but rather the first moment of a **probability distribution**. However, this research focused on the differences resulting from the CI or IC methods, also acknowledging that in practice decision making processes would hardly incorporate complete uncertainty analysis e.g. through Monte Carlo simulations.

Finally, in the context of **decision making**, the CA approach has to be taken into account if spatial output is not required. This study showed that the **differences between CI or IC will be overcome if the user chooses a non-spatial approach**, based on the available point information. This is because any real-case study that involves the interpolation of environmental variables from point information will almost certainly find some **nugget effect** and **hence a reduction in the heterogeneity** during interpolation.

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