Impact of short range variability of soil and substance properties on regional scale atrazine exposure to groundwater

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Objective and methodology

Pesticide exposure to groundwater at the regional scale can be assessed by different modeling approaches. Meta-models, are a good compromise since they are calibrated on conceptual physical based models and they intrinsically behave as the fully conceptual model. Unfortunately, groundwater exposure modeling at the regional scale remains subjected to many sources of uncertainty and it is the uncertainty that limits the use of regional scale exposure modeling into practical decision making (Dubus, Brown and Beulke 2003). This study presents uncertainty propagation aspects when modeling exposure of atrazine to groundwater by means of MetaPEARL (Tiktak et al., 2006) in a hydrological catchment in the South of Belgium. We use particularly the MetaPEARL version which was calibrated on the EuroPEARL model, a pan European implementation of GeoPEARL (Tiktak et al. 2004).

Using MetaPEARL and ignoring extraction of pesticides in the root zone of agricultural crops, predicted environmental concentration of a pesticide, PEC (µg/l), can be calculated by:

$$PEC = \exp\left(\alpha_0 - \alpha_1.X_1 - \alpha_2.X_2\right) \qquad X_1 = \frac{\mu.\theta.L}{q} \qquad X_2 = \frac{\mu.\rho.OM.Kom.L}{q}$$

with, µ (day^{-1}), the first order degradation rate of the pesticide, where µ = ln(2)/DT50 and DT50 (day), the pesticide half live; θ (-), the volumetric soil moisture content; L (m), the depth from the soil surface to the groundwater table; q ($m\ day^{-1}$), the groundwater recharge flux; ρ ($kg\ dm^{-3}$), the soil bulk density; OM ($kg\ kg^{-1}$), the organic mater content and Kom ($dm^3\ kg^{-1}$) the organic matter sorption coefficient; and α_0, α_1 and α_2 empirical calibration constants. In this case study, L was fixed at 1 m depth.

The case study: The Molignée catchment

The Molignée catchment is situated in Condroz region, in the South of Belgium (figure 1). The catchment has a total area of 7611 ha. The climate is temperate humid, with mean annual precipitation of 924 mm and mean annual temperature of 8-9°C. The main soil types (fig. 2) encountered in the catchment are loamy-stony soils with micaceous sandstone load (30 % of the catchment) on the crests and loamy-stony soils with limestone load (20 %) in the calcareous depressions. Main land use is meadow land (30%) followed by wheat (20 %), barley (15 %), sugar beet (6 %) and maize (5 %) crop land.

Fig. 1. Situation of the study catchment in Belgium.

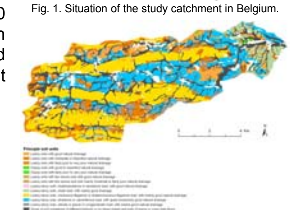
Fig.2. Principle soil units within the study region.

Deterministic regional scale assessment for atrazine exposure

We first implemented a deterministic (i.e. ignoring uncertainty on model parameters) but spatially distributed modeling approach, considering soil related parameters of MetaPEARL (ρ, OM, θ, L) being spatially distributed. Use was made of the regional soil map published at the scale of 1:250.000 (Bah and Bock, 2006). Within the study region, agricultural land use is represented by 5 principle soil types characterized by soil analytical data. Summary soil profile data are given in Table 1. MetaPEARL model was evaluated for a hypothetical autumn application of atrazine on winter wheat crop. For the reference simulation a DT50 = 61 days, and Kom = 74 $dm^3\ kg^{-1}$ was imposed. The parameters α_0, α_1 and α_2 were set equal to 4.95, 0.16, 0.60 respectively. The corresponding PEC is shown in figure 3.

Table 1. Summary soil profile data and deterministic PEC (µg/l) prediction for atrazine

Soil type	Percentage of surface area	% Clay	% Loam	% Sand	% organic C	PEC (µg/l)
Aba /AbB	9,3	21,33	72,16	6,51	0,40	0,532
Ghxf4	4,3	24,61	54,11	21,25	0,78	0,007
Gbbp0_1	29,2	19,97	41,84	38,16	0,76	0,010
GbBK0_1	18,1	40,83	44,72	14,42	0,74	0,014
Gbax2	3,7	15,77	17,78	66,49	0,42	0,787

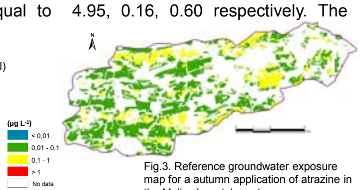

Fig.3. Reference groundwater exposure map for a autumn application of atrazine in the Molignée catchment

Results

The deterministic PEC (table 1) varies between 0.007 and 0.787 ppb. As expected, the highest PEC is calculated for the Gbax2 soil which is low in organic matter (0.42%) and highest in sand content (66 %). As well Gbax2 as Aba/AbB, with low organic matter content (< 0.42%), yield PEC values which largely exceeds the drinking water norm of 0.01 ppb. Yet, these soil types represent only 13 % of the total catchment area. 51 % of the catchment area has a PEC which is slightly lower or close to the drinking water norm. This confirms the vulnerability of groundwater to atrazine exposure.

The consideration of uncertainty on DT50 (table 3) has little effect on the median PEC. Yet, some difference between median and deterministic PEC is introduced, when using the lognormal DT50 pdf in the stochastic simulation, in particular for the most vulnerable soil types (Aba/AbB and Gbax2). In contrast to the median PEC and as expected, percentile PEC is largely affected by the uncertainty on DT50. We conclude therefore that it is important to consider variability of DT50 and that percentile PEC are more relevant from a risk point of view.

The variable OM has apparent low impact on median PEC (table 4) when vulnerability is already high (Aba/AbB and Gbax2 soil). However, median PEC increases between one and two orders of magnitude for lower vulnerable soils, suggesting that the exposure model is highly non linear in the proposed OM variability range. As expected, OM variability has significant effect on PEC percentiles, with an increase of nearly 2 orders of magnitude when variation coefficients of 100 % for OM are considered for all soils.

As compared to DT50 and OM, much less sensitivity of θ variability on PEC is observed.

Considering a joint variability of DT50, OM and θ is slightly sensitive for median PEC and, as expected, significantly sensitive for the percentile PEC.

Table 4. Table 4. Deterministic and stochastic PEC (µg/l) prediction for variable OM (scenario 4, 5 and 6).

		Median value			80th Percentile value		
Soil type	Deterministic DT50 = 61 days	Stochastic (CV = 10%)	Stochastic (CV = 40%)	Stochastic (CV = 100%)	Stochastic (CV = 10%)	Stochastic (CV = 40%)	Stochastic (CV = 100%)
Aba /AbB	0,532	0,532	0,532	0,527	0,794	2,663	31,980
Ghxf4	0,007	0,546	0,546	0,540	0,815	2,730	32,774
Gbbp0_1	0,010	0,592	0,592	0,586	0,884	2,961	35,526
GbBK0_1	0,014	0,591	0,591	0,585	0,869	2,774	30,073
Gbax2	0,787	1,010	1,010	1,000	1,464	4,489	44,639

Uncertainty analysis

Uncertainty analysis focused on uncertainty propagation of DT50 (61 days), organic matter and soil moisture content and was performed using Monte Carlo simulation method. Joint probability density functions (pdfs) of these three parameters were reconstructed and 1000 samples were drawn from the reconstructed pdfs in a stratified way using the latin hypercube sampling procedure. Initial trials showed that 1000 samples were largely sufficient to get stable PEC values. In addition to the reference scenario (scenario 1), 11 uncertainty analysis scenarios (scenario 2 to 12) were considered. A summary of the scenarios is given in Table 2. Scenario's 2-3 dealt with uncertainty on DT50, which is very sensitive in PEC assessments, but also very uncertain. The cumulative frequency distribution of observed data (Dorgelo, 2006) on a lognormal scale is given in figure 4. Scenario's 4-6 dealt with uncertainty on OM. OM determines the sorption behaviour of the soil and is generally considered as very sensitive soil parameter in PEC assessment. To cover potential ranges of OM variability, scenarios 4-6 corresponds to 3 levels of variation of 10 %, 40 % and 100 % respectively.

Scenarios 7-9 dealt with uncertainty on θ. It is expected that uncertainty of θ is less sensitive, though its variability within the field can be very high. to cover potential ranges of θ variability, scenarios 7-9 consider 3 levels of variation of θ of 20 %, 40 % and 60 % respectively. Finally scenario 10-12 considers the impact of the joint variability of DT50, OM and θ. In scenario 10, no correlation between parameters is considered. In scenario 11 and 12 opposite correlation (correlation coefficient of +0.6 and -0.6 resp.) between DT50 and OM is considered.

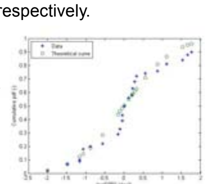
Fig.4. Cumulative frequency distribution function of observed DT50 data (Source: Dorgelo, 2006).

Table 3. Deterministic and stochastic PEC (µg/l) prediction for variable DT50 (scenario 2 and 3).

		Median value		80th Percentile value	
Soil type	Deterministic DT50 = 61 days	Stochastic DT50 lognormal transformed	Stochastic DT50 integral transformed	Stochastic DT50 lognormal transformed	Stochastic DT50 integral transformed
Aba /AbB	0,532	0,545	0,532	3,461	1,154
Ghxf4	0,007	0,007	0,007	0,190	0,027
Gbbp0_1	0,010	0,010	0,010	0,239	0,036
GbBK0_1	0,014	0,014	0,014	0,303	0,049
Gbax2	0,787	0,805	0,787	4,488	1,616

Table 2. Scenarios considered in the uncertainty propagation analysis.

Scenario-ID	Stochastic parameter	Distribution type	Coefficient of variation (%)	Correlation structure
1	None	None	None	None
2	DT50	Lognormal	Fitted to data (see figure)	None
3	DT50	Integral	Fitted to data (see figure)	None
4	OM	Normal	10	None
5	OM	Normal	40	None
6	OM	Normal	100	None
7	θ	Normal	20	None
8	θ	Normal	40	None
9	θ	Normal	60	None
10	DT50/OM/θ	Cf. scenario 3, 5, 8	Cf. scenario 3, 5, 8	None
11	DT50/OM/θ	Cf. scenario 3, 5, 8	Cf. scenario 3, 5, 8	DT50-OM: positif
12	DT50/OM/θ	Cf. scenario 3, 5, 8	Cf. scenario 3, 5, 8	DT50-OM: negatif

Conclusion

- The deterministic simulation suggests that most of the agricultural area in the catchment is indeed susceptible to groundwater exposure from atrazine. PECs exceed the drinking water limit, but with strong differences of susceptibility between the different soil types. The vulnerability is well correlated with the estimated organic matter in the soil profile.
- The stochastic simulation of median PEC seems to be strongly influenced by the adopted variability of OM, less by DT50 and not by θ, suggesting important non-linearity of the exposure model in the OM range, in particular when the vulnerability of the soils is low or close to the drinking water limit endpoint.
- The uncertainty components of individual factors seem further to be partially additive when considering the joint uncertainty. Therefore, the joint uncertainty should be analysed and due attention should be devoted to the reconstruction of the correlation structure underlaying factors.