COMPARISON OF GEOPEARL WITH THE SINGLE SCENARIO APPROACH IN PESTICIDE REGISTRATION

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ABSTRACT
Several countries use one or a few scenarios to evaluate the leaching of pesticides. This, however, can be too strict for some substances while being too lenient for others, because of the wide ranges in pesticide properties. In a GIS approach the variability is explicitly taken into account and more accurate results are expected. This research has been carried out to compare the two approaches.
The PEARL model was used to calculate the leaching in 8 FOCUS scenarios and the Dutch standard scenario (NLS). A number of pesticides was included, covering wide ranges in properties. The spatially distributed model GeoPEARL was used to calculate the 90th percentile leaching concentrations for the Netherlands, taking into account information on a.o. soil properties and climatic conditions.
None of the scenarios is capable of representing realistic worst-case conditions in the Netherlands for the broad range of pesticides. Six FOCUS scenarios appear to be more vulnerable. Using the FOCUS approach, the NLS and GeoPEARL results agree well, except for volatile and acidic substances. When using single applications, NLS-results appear to be lower: the ratio (GeoPEARL/NLS) ranges from 1 to 385. We conclude that tools such as GeoPEARL should replace single scenarios in evaluation studies.

KEYWORDS: GIS, Groundwater, Leaching, Modelling, Scenario

INTRODUCTION

Contamination of groundwater is an important side effect of the usage of plant protection products (PPPs) in agriculture. Leaching to groundwater therefore is one of the key elements in the registration procedures at both the European level (EU, 1991; EU, 1997; FOCUS, 2000) and the level of individual member states (e.g. Brouwer *et al*., 1994; Resseler *et al*., 1997). PPPs can not be registered if the expected leaching concentration of the parent substance, or of its relevant metabolites, under realistic worst case conditions exceeds the threshold level of 0.1 μg dm^{-3}. Registration procedures follow a tiered approach. In these procedures the risk of usage of PPPs for man and environment is evaluated in a number of sequential steps, taking into account more detailed or more specific information in each following step. In the first tier of the leaching assessment at the European level, point scale exposure models are used in combination with single standard scenarios (FOCUS, 2000). In the Netherlands a comparable approach is followed. The point scale PEARL model (Tiktak *et al.*, 2000; Leistra *et al.,* 2001) is used in combination with a single scenario (Boesten and Van der Linden, 1991) to assess predicted environmental concentrations (PECs). A scenario consists of a combination of soil, climate and crop parameters. Standard scenarios increase the consistency of the regulatory process by minimising the subjective influence of the person who performs the evaluations. In the registration procedure, the standard scenario should represent realistic worst case conditions (EU, 1991; FOCUS, 2000). Van der Linden *et al.* (2003) propose to use the 90% vulnerable location as the realistic worst case condition, which implies that the PEC of a PPP should be less than the EU drinking water limit in at least 90% of the area where it is potentially used.

The selection of the Dutch standard scenario (NLS) was based on expert judgement and not on statistical approaches (Boesten and Van der Linden, 1991). It is therefore not clear whether these soil, crop and management conditions are true representatives of the 90th percentile vulnerable location. Spatially distributed models like GeoPEARL (Tiktak *et al*., 2002a) can provide an answer to this question. These models provide the user with maps of the leaching concentration in an entire region. Frequency distributions and percentiles of the leaching concentration can directly be inferred from these maps. These percentiles can directly be compared with the PEC obtained with the single scenario approach.

The objective of this paper is to evaluate whether it is possible to use a single standard scenario to describe realistic worst case conditions. For the full range of possibly registered PPPs, the 90th percentile of the leaching concentration as inferred from a spatially distributed model is compared with results from the single scenario approach. A total number of nine scenarios is evaluated for Dutch conditions, i.e. the NLS (Boesten and Van der Linden, 1991) and eight FOCUS groundwater scenarios (FOCUS, 2000). The comparison will be made for a number of PPPs, together covering wide ranges in physico-chemical properties. The consequences for the pesticide registration procedures will be discussed. This paper focuses on the Dutch situation; the applicability of the FOCUS scenarios for the EU registration procedure is evaluated in a separate paper (Tiktak *et al*., 2003).

METHODS

A systematic comparison is made between results from the 'single scenario approach' and results from a spatially distributed model. The target variable is the predicted leaching concentration, also referred to as the PEC groundwater. For the 'single scenario approach' the Dutch standard scenario (NLS) was used. To obtain the predicted leaching concentration with the NLS, the PEARL model was used. PEARL is a one-dimensional, dynamic, multi-layer model of the fate of a PPP and relevant transformation products in the soil-plant system. The model is linked with the Soil Water Atmosphere Plant (SWAP) model. Tiktak *et al*. (2000) and Leistra *et al*. (2001) give a comprehensive overview of the PEARL model. The SWAP model is described by Van Dam (2000). The spatially distributed model adopted in this study was the GeoPEARL model (Tiktak *et al.*, 2002a).

For the NLS, a well-drained sandy soil was selected (Boesten and Van der Linden, 1991). This soil is low in organic matter (c. 1.6 % over the top metre), the *p*H is around 4.6 and the groundwater table is at a depth of approximately 1 m. The soil is covered with a maize crop during the growing season and fallow in winter. Also, weather data from a single rather wet year – 75th percentile year of the total precipitation amounts - were used. For simulation periods exceeding one year, the climatic conditions are repeated. The combination of this soil – approximately 80th percentile in vulnerability - with the selected weather data was believed to constitute a reasonable worst case situation. The current Dutch registration procedure prescribes to use a single surface application. The target variable of the calculations is the maximum average concentration in the uppermost metre of the groundwater. In the proposed new Dutch registration procedure (Van der Linden *et al*., 2003), the European practice will be adopted (FOCUS, 2000). In this methodology, the simulation period is 26 years, of which the first six years are considered to be a 'warming-up' period. Also, the application is repeated every year. The target variable in this calculation is the 80th percentile in time of the annual leaching concentration. Again, the combination of the relatively vulnerable soil and the 80th percentile in time is believed to constitute a reasonable worst case, i.e. a 90th percentile in vulnerability. Both the new and the old procedure were used in this exercise; for the long-term weather series data for the period 1975 – 2000 from weather station De Bilt in the Netherlands were used (same station as for the NLS).

In addition to the NLS, eight FOCUS scenarios were selected with maize as the growing crop; so all locations except Jokioinen (FOCUS, 2000). The 80th percentile concentrations in time were used for this comparison exercise. The results for these scenarios are compared to the results obtained for the NLS and the GeoPEARL simulations.

The spatially distributed model used in this paper is the GeoPEARL model (Tiktak *et al.*, 2002a). GeoPEARL is basically a combination of the local-scale PEARL model with a Geographical Information System. To describe the interaction with the local and regional groundwater system correctly, the model was loosely coupled with a regional groundwater model. Calculations can be performed for 6405 so-called plots, which are unique combinations of spatially distributed model inputs. The unique combinations were obtained by combining in a GIS maps of the most important spatially distributed model inputs, i.e. soil type, crop type, weather district and hydrotype. The latter is an entity describing the local groundwater system (Kroon *et al.*, 2001). Before the overlay was created, all maps were converted to raster maps with a resolution of 250x250 m^2. The size of the unique combinations is between 0.25 km^2 and 220 km^2, with a median size of 3 km^2. For each individual plot, the calculation procedure was essentially the same as in the FOCUS procedure, i.e. a 26 years simulation period and the application repeated every year. The target variable in the GeoPEARL calculations is the 50th percentile concentration in time of the location representing the 90th percentile in vulnerability of the area (Van der Linden *et al.*, 2003). First, the median of the leaching concentrations for each plot over 20 years is calculated. After this, the 90th percentile of the median concentrations for all plots is determined.

GeoPEARL has options to reduce the number of unique combinations. This largely reduces the computation time, which is beneficial when simulations must be carried out for a large number of substances. For most substances a good approximation is obtained when the number of scenarios is reduced to 250 (Tiktak *et al.*, 2002b). This option was chosen in the present study for all hypothetical substances.

The substances used in this study are a combination of 18 hypothetical substances and 21 real substances that were registered in the Netherlands in the past. The hypothetical substances were added to ascertain a wide variety of physico-chemical properties with respect to transformation and sorption coefficients. Transformation half-life for parent substances ranged from 1 to 200 days, while the coefficient for sorption on organic matter ranged from 0 to 200 dm^3 kg^{-1}. Two metabolites were included, which have a half-life of approximately 3 years. The real substances included also moderately and highly volatile substances (for example the soil disinfectant 1,3-dichloropropene) and substances showing pH-dependent sorption behaviour (for example dinoseb). The hypothetical substances were non-volatile: the vapour pressure was set to zero. All hypothetical substances were applied at a net dosage of 1 kg ha^{-1} to the soil surface. For the other substances application techniques included injection (highly volatile substances) and incorporation (moderately volatile substances) and application rates differed from 0.1 to 100 kg ha^{-1}, approximating agricultural practice. For easy comparison, results were calculated back to a standard application of 1 kg ha^{-1} by assuming linear response of the leaching concentration to the application rate.

RESULTS AND DISCUSSION

The FOCUS scenarios and the NLS are used to evaluate the leaching within the framework of the registration of plant protection products. The scenarios were derived to represent realistic worst case situations for major agricultural areas in Europe and for the total agricultural area in the Netherlands, respectively. In the framework of FOCUS, realistic worst case is defined as the 90th percentile vulnerable situation (FOCUS, 2000), with vulnerability attributed in equal shares to soil and climatic conditions. In the Netherlands, the most important consideration is to protect the groundwater as a source of drinking water, so a slightly different approach is adopted (Van der Linden *et al.*, 2003). As the extracted water is a mixture of the rainfall surplus of many years, it is preferable to protect a large area on long-term, rather than a small area against peak concentrations. Consequently, it was decided to use the overall 90th percentile in terms of the surface area on which a PPP is (potentially) used, and median climatic conditions.

Table 1. Calculated concentrations (μg dm^{-3}) for hypothetical substances in groundwater for FOCUS scenarios, the NL scenario and the GeoPEARL approach (< denotes a concentration <0.0005 μg dm^{-3}).

DT50	Kom	Location#					
d	$dm^3\ kg^{-1}$	C	H	K	N	NLS_0*	GeoPEARL
5	5	0.005	0.038	0.024	0.034	<	0.001
5	8	0.001	0.011	0.008	0.016	<	<
5	12.5	<	0.001	0.001	0.005	<	<
10	10	0.157	0.487	0.323	0.798	0.007	0.055
10	17	0.031	0.119	0.084	0.288	0.001	0.009
10	25	0.005	0.027	0.014	0.071	<	0.001
20	20	1.227	2.478	1.799	3.050	0.222	0.496
20	33	0.238	0.398	0.281	0.746	0.020	0.081
20	50	0.024	0.038	0.028	0.087	<	0.003
40	67	0.408	0.823	0.569	0.857	0.014	0.078
50	50	3.883	4.931	3.830	5.706	0.360	1.270
50	125	0.032	0.076	0.047	0.095	<	0.003
80	130	0.627	0.999	0.696	1.103	0.011	0.097
80	200	0.036	0.074	0.048	0.082	<	0.003
100	100	4.88	6.379	4.587	6.587	0.246	1.470
120	200	0.611	0.853	0.634	0.949	0.005	0.088
150	150	5.364	6.286	5.139	6.684	0.162	1.400
200	200	5.673	6.528	5.217	6.823	0.115	1.520

C Chateaudun, H Hamburg, K Kremsmünster, N Okehampton, NLS Dutch standard scenario

* NLS_0 Results calculated for a single application

Table 1 gives the leaching concentrations (the target variable) for selected hypothetical substances as obtained in the calculations for the single scenarios and for the GeoPEARL calculations. Results for the FOCUS scenarios C, H, K and N are also listed, because these are considered to be the most relevant scenarios for the Dutch conditions. It can be easily observed that the results obtained with GeoPEARL are all above the results for the NLS. Also, the simulated concentrations in the four FOCUS scenarios are all above the 90th percentile of the GeoPEARL calculations and far above the results for the NLS. Results for the other four FOCUS scenarios are not shown, because the climatic conditions of these scenarios are considered less relevant for the temperate climate of the Netherlands. The results obtained for the T (Thiva) and P (Piacenza) scenarios are in line with the results shown. In contrast, concentrations simulated for the S (Sevilla) and O (Porto) scenarios are lower than for the NLS and GeoPEARL calculations. So, for spring and early summer applications six out of eight FOCUS scenarios appear to be more vulnerable than the 90th percentile situation in the Netherlands. This conclusion only applies to non-volatile substances that have a surface application and for which the behaviour in soil can be described according to first order kinetic transformation and sorption proportional to the organic matter of the soil.

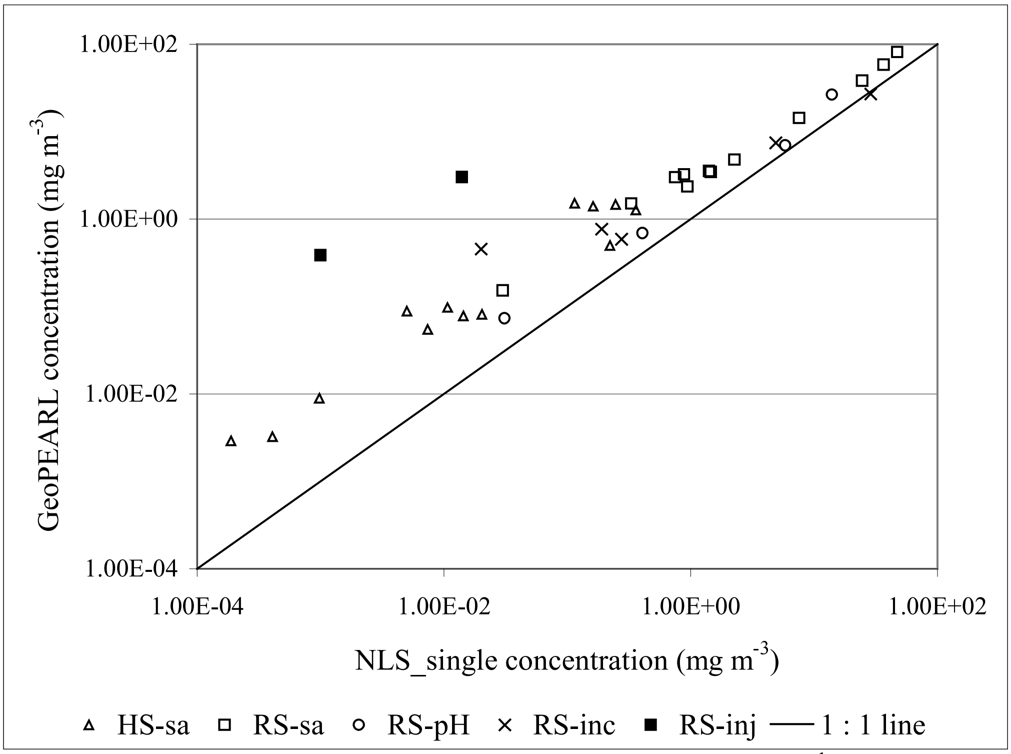

Figure 1 Comparison of NLS concentrations (single application) and 90th percentile GeoPEARL concentrations. HS: hypothetical substance, RS: real substance, sa: surface applied, pH: pH-dependent sorption, inc: incorporated, inj: injected.

To explore whether the GeoPEARL produces higher PECs for other application techniques and substances with other physico-chemical properties as well, additional calculations were performed for a number of substances that were registered in the past. Figure 1 gives the results of the calculations for both the hypothetical and the selected real substances. Very low calculated concentrations (< 1E-4 µg dm^{-3}) are not shown for various reasons: the calculations at such low concentration are not very accurate, such low concentrations are not critical in decision making and inclusion would render an illegible graph.

Concentrations obtained for the NLS are always lower than the 90th percentile concentrations obtained with GeoPEARL, except for the second metabolite of aldicarb (aldicarb-sulphone) for which the ratio of the calculated concentrations is 0.9. For the other non-volatile substances the ratios GeoPEARL (90th percentile) / NLS_0 range from 1.2 to 30 (median value is 4). For two highly volatile substances the ratio is 215 and 385 respectively. In the NLS in this case the pH of the soil was assumed to be 7, so relatively worst case. Still then the leaching appears to be lower.

From Table 1 it appears that the NLS is not representative of the 90th percentile vulnerable situation in the Netherlands. However, except for the different number of scenarios that were considered, two major changes in the calculation procedure were adopted at the same time: 1) a single application versus repeated applications, and 2) a single year of weather data versus a 26 year time series of weather data. Figure 2 compares the results of the calculations with GeoPEARL to the results obtained with the 80th percentile concentration of the long-term NLS calculations (FOCUS approach, annual application). For most substances, there is a rather good agreement in the results. Rather large deviations are found for the highly volatile substances, which are injected in the soil and for substances with pH dependent sorption.

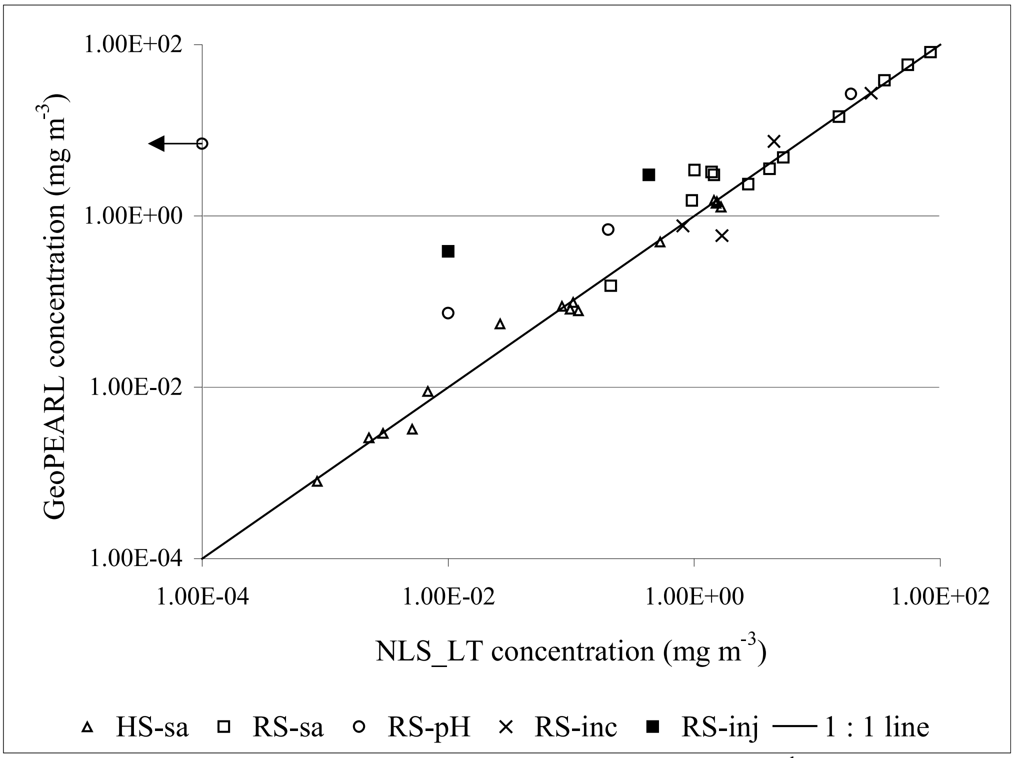

Figure 2 Comparison of NLS concentrations (FOCUS method) and 90th percentile GeoPEARL concentrations. HS: hypothetical substance, RS: real substance; sa: surface applied, pH: pH-dependent sorption, inc: incorporated, inj: injected.

The rather large differences for the soil disinfectants can be attributed to differences in the groundwater depth, which highly influences the transport of the substances in the gas phase (Tiktak *et al.*, 1996). In situations with a very shallow groundwater table, less substance volatilises to the atmosphere and calculated concentrations in the groundwater will be higher. In areas with such high groundwater levels many soils will have artificial drainage and substances may largely end up in the surface water and volatilise from there. This process is relevant for substances having a dimensionless Henri coefficient above 10^{-5}.

In Figure 2 the soil-pH of the NLS was set to the original value, which is around 4.6 (Boesten and Van der Linden, 1991). For dinoseb a very low leaching level (around 1E-10 μg dm^{-3}) is calculated for the NLS (indicated with the arrow in Figure 2); the difference with the GeoPEARL concentration being approximately 10 orders of magnitude. For the other three substances showing pH dependent sorption, the differences are much smaller. This can be attributed to lower pK_a values for these substances (around 3 or lower, dinoseb 4.62). At the pH of the standard soil, approximately 50% of dinoseb is dissociated and the neutral molecule and the anion contribute in equal shares to the sorption. For the other three substances the dissociated form dominates (more than 95%). In nearly all agricultural soils the sorption of these substances will be rather low and the height of the groundwater table has more influence than the sorption constant.

Additional calculations with repeated applications to the NLS, but with a single year of weather data (repeated 26 years) showed results comparable to the results obtained for the calculations with the long term weather data (data not shown). Apparently the repetition of the application has a larger influence than the differences in weather data between the years.

For most substances the NLS, operated conform the FOCUS approach, seems to represent the reasonable worst case for the Netherlands quite good. However, for the highly volatile and dissociating substances differences in calculated leaching for the reasonable worst case condition may become quite large. For the dissociating substances the disagreement becomes larger when the pK_a of a substance is in the range of the pH values of agricultural soils, i.e. is between 4 and 8. As the number of dissociating PPPs and metabolites is quite large, it is very important to take this into account in the evaluation procedure. A single scenario hardly ever represents the reasonable worst case for these substances.

This study compares the leaching for substances applied in spring. It is expected that approximately the same results will be obtained for applications in other seasons.

CONCLUSIONS

One of the aims in the Netherlands is to protect the groundwater as a source of drinking water. To achieve this goal, it has been proposed to use the 'reasonable-worst-case-criterion' in terms of the surface area on which a PPP is (potentially) used, and median climatic conditions. The current Dutch procedure underestimates the leaching risk of PPPs when compared to results of a spatially distributed model.

When following FOCUS calculation procedures, the NLS is quite representative of the reasonable worst case leaching conditions for ordinary substances, but fails for highly volatile and dissociating PPPs. It will be impossible to find a single scenario that represents the reasonable worst case situation for the broad ranges in physico-chemical properties of PPPs. The leaching of pesticides is highly sensitive to scenario characteristics (soil, hydrology and weather). It is therefore crucial to evaluate leaching using a procedure that includes geographical information. The approximating procedure, based on a single scenario, may give deviating results up to even more than two orders of magnitude.

For hypothetical substances six FOCUS scenarios proved to be more vulnerable than the 90^{th} percentile situation in the Netherlands, for ordinarily behaving substances. For highly volatile and dissociating substances, these scenarios will face exactly the same problems as the NLS; a single scenario here cannot be representative of the highly variable circumstances in agricultural soils. Further work, however, has to reveal whether one or more of these scenarios can play a role in the registration process in the Netherlands.

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