Estimation of pesticide parameters from static and dynamic experiments by two independent modelling groups

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ABSTRACT

The behaviour of a pesticide was tested in laboratory, micro-lysimeter, field lysimeter and field dissipation studies. Field lysimeter data were used by two independent modelling groups for estimating Koc and DT50 values. DT50 values derived from dynamic systems (micro-lysimeter, lysimeter) were shorter than those in static laboratory studies. Optimised Koc values differed somewhat between modelling groups and methods, due to differences in the approach to calibration. Total residues in independent field studies were better simulated with parameters derived from dynamic than static systems.

INTRODUCTION

Degradation and sorption parameters to predict the environmental behaviour of pesticides are traditionally determined in static laboratory studies. These parameters may not always be applicable to field conditions (Beulke *et al.*, 2000). The behaviour of a compound (denoted Y) was tested under static and dynamic conditions and at different scales in laboratory incubation, batch equilibrium, micro-lysimeter, lysimeter and field dissipation studies. A subset of these studies was used by two independent modelling groups for automatic and manual parameter estimation. The suitability of these parameters to predict the behaviour of compound Y under different environmental conditions was evaluated.

EXPERIMENTAL STUDIES

DT50 values in soil (the time for 50% dissipation of the pesticide), K_{OC} values (sorption coefficients normalised to soil organic carbon content) and n_f values (Freundlich exponents) were derived from static laboratory degradation and sorption studies with the test substance for a number of soils (Table 1).

Table 1.   Properties of test compound Y in laboratory experiments

	DT50 (days)[1]	Koc (l/kg)	nf
No. of studies	6	21	19
Minimum	22	17.0	0.76
Maximum	59	109.0	1.00
Average	40	39.3	0.92
Median	37	32.5	0.94

[1] at 20°C and 40% maximum water-holding capacity

DT50 values ranged from 22 to 59 days with an average of 40 days. Average values for K_{OC} and nf were 39.3 dm³/kg and 0.92, respectively. For three soils (sandy loams A and B, loam C), data were available for more than one type of experiment. Batch sorption and micro-lysimeter studies were performed with all three soils and sandy loam A was also used in the field lysimeter study. Batch sorption data (K_{OC}/nf) for sandy loam A, sandy loam B and loam C were 30 l/kg / 0.91, 28 l/kg / 0.94 and 23 l/kg / 0.93, respectively.

Three replicate micro-lysimeter studies were performed under controlled conditions with undisturbed topsoil (0-28 cm) to get an insight into the leaching and degradation behaviour of compound Y under conditions closer to the field. The micro-lysimeters were irrigated at an average infiltration rate of 3.4 mm/day during a 100-day study period. Degradation and sorption parameters of compound Y in sandy loam A (Table 2) were derived from breakthrough curves with CXTFIT-2.1 (Toride *et al.*, 1995) assuming linear sorption (nf = 1). Where amounts leached were too small to obtain reasonable fits (sandy loam B, loam C), DT50 values were calculated from the mass balance.

Table 2. Sorption and degradation of compound Y in undisturbed soil columns

Soil	Amount of Compound Y (% of applied)			K_{OC} from BTC (l/kg)	DT50 at 20°C (days)
	Soil	Leachate	Dissipated		
sandy loam A (rep. 1)	1.3	47.3	51.4	20	14 [a]
sandy loam A (rep. 2)	-	-	-	22	16 [a]
sandy loam A (rep. 3)	-	-	-	21	7 [a]
sandy loam A (mean)	-	-	-	22.1	12.2
sandy loam B	6.9	0.6	92.5	>> 50	20 [b]
loam C	1.3	0.8	97.9	>> 50	< 7 [b]

[a] DT50 and K_{OC} estimated simultaneously from the BTC (=breakthrough curve) with CXTFIT-2.1.
[b] DT50 estimated from the applied and residual mass of compound Y in the soil column and the mass in leachate assuming first-order decay.

Dissipation of compound Y in field studies was investigated under a range of environmental conditions (5 studies in Europe, average air temperatures 14.0-19.1°C; 3 studies in the US, 11.5-16.6°C; 3 studies in Canada, 3.4-7.7°C). In Europe, sampling started in spring after a single application and continued until residues fell below the limit of quantification (usually <100 days). Multiple applications were made in the US and Canada. Samples were taken up to >360 d after the last treatment in September. Field dissipation rates were corrected to degradation rates at the reference temperature for a standardised evaluation and comparison with laboratory values at 20°C using the relationship

$$k_{act} = k_{ref. at 20°C} \; Q_{10}^{\frac{T-20}{10}}$$

with k_{act} = measured degradation rate in the field (1/day), $k_{ref\ at\ 20°C}$ = standardised degradation rate at 20°C (1/day), Q10 = factor of change in degradation for a change in temperature by 10°C (fixed at 2.2) and T = measured daily temperature (°C).

Daily degradation rates were calculated with the ModelMaker program using measured daily temperatures. The degradation rate at the reference temperature was optimised for best fit to the experimental data. First-order DT50 values obtained with and without temperature correction are listed in Table 3.

Table 3. Field DT50 values of compound Y (measured and corrected to 20°C)

Site	Application time/ sampling period	Average temperature (°C)	DT50 (days)	DT50 at 20°C (days)
EU1	spring / <100 d	17.7	14.2	11.7
EU2	spring / <100 d	19.1	7.3	6.3
EU3	spring / <100 d	14.0	37.5	27.6
EU4	spring / <100 d	16.6	4.9	5.8
EU5	spring / <200 d	16.7	22.2	13.2
US6	autumn / >360 d	13.5	19.6	13.1
US7	autumn / >360 d	11.5	12.8	10.1
US8	autumn / >360 d	16.6	7.1	8.7
CAN9	autumn / >360 d	7.7	25.6	15.0
CAN10	autumn / >360 d	8.8	15.4	11.7
CAN11	autumn / >360 d	3.4	54.4	17.5
Minimum – Maximum			4.9 – 54.4	5.8 – 27.6
Arithmetic mean (Median)			20.1 (15.4)	12.8 (11.7)

The field first-order DT50 values were more scattered (5-54 d) and the distribution was more skewed than the DT50 values standardised to 20°C (6-28 d).

A lysimeter study was performed over 3 years according to the German lysimeter guideline (soil = sandy loam A). Application to two replicate lysimeters (B and C) was made in the first year only, whereas a third lysimeter (A) received applications in year 1 and 2. Annual average concentrations in the leachate from individual lysimeters were below 0.1 μg/l (< 0.001 to 0.04 μg/l).

PARAMETER ESTIMATION FROM FIELD LYSIMETER STUDIES

The sensitive parameters K_{OC} and DT50 were estimated from the breakthrough curves of compound Y in leachate from field lysimeters either by (i) automatic calibration of PESTRAS (Freijer *et al.*, 1996) by inverse modelling using a Simplex procedure which aimed at minimising the sum of squared residuals (modelling group A) or (ii) automatic calibration of PEARL (Tiktak *et al.*, 2000) by inverse modelling using a Marquardt-Levenberg procedure (group B) or (iii) manual calibration of PEARL using expert judgement and visual fit to estimate suitable parameters (group B).

The hydrology of the lysimeters was first calibrated by adjusting evapotranspiration within reasonable limits. This was achieved by modifying leaf-area indices of the crops (group A) or by changing crop-specific evapotranspiration factors, leaf-area indices and factors for bare-soil evaporation (group B). Thereafter, Koc and DT50 values were calibrated to improve the fit to concentrations of compound Y in the lysimeter leachates (Figures 1a and 1b). Optimised parameters obtained by the two groups are given in Table 4. The automatic calibration by group B yielded different optimised Koc and DT50 values depending on parameters not included in the calibration and, in contrast to group A, depending also on the starting values.
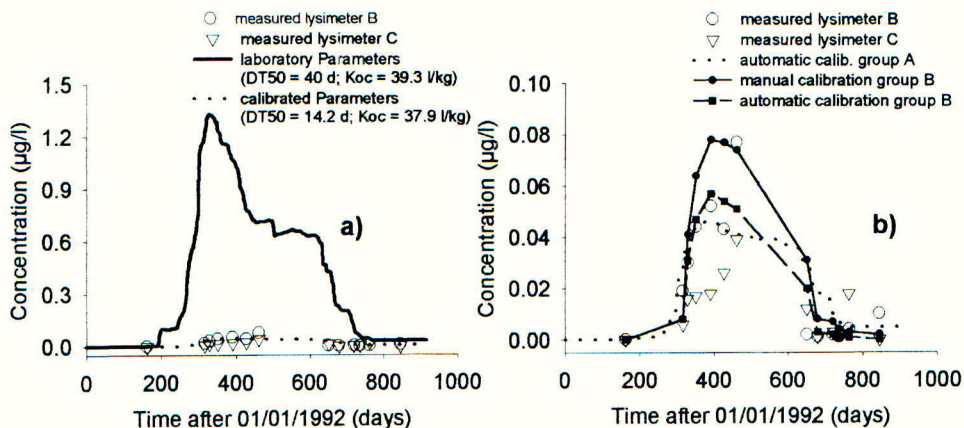
Figure 1 Measured and simulated concentrations of compound Y in lysimeters B and C using initial and calibrated parameters (a) and parameter combinations calibrated by the two modelling groups (b)

Table 4. Optimised parameters obtained from the lysimeter study

Lysimeter	DT50 (days)				K_{OC} (l/kg)			
	A	B	C	Mean	A	B	C	Mean
Group A automatic	14.4	14.8	13.4	14.2	40.2	35.7	37.8	37.9
Group B automatic		9.8				12.4		
Group B manual		14.0				19.5		

A substantial improvement of the simulated breakthrough curve compared to measurements could be obtained by all optimisations. The differences between the optimised are small compared to the range of parameters obtained in static laboratory systems.

COMPARISON OF PESTICIDE PARAMETERS FROM DIFFERENT STUDIES

Degradation parameters obtained in the dynamic systems (micro-lysimeter, field study and field lysimeter study) were similar (Table 5), irrespective of the parameter estimation technique and the modelling group.

Table 5. Pesticide parameters for compound Y obtained from different experiments

	Static system	Dynamic systems				
	Laboratory	Micro-lysimeter (*sandy loam A*)	Field dissipation (average)	Lysimeter		
				Group A (autom.)	Group B (autom.)	Group B (manual)
DT50 (d)	40	12.2	12.8	14.2	9.8	14.0
K_{OC} [l/kg]	39.3	22.1	-	37.9	12.4	19.5

The difference between the optimised values is small compared to the range of parameters obtained in static laboratory systems. The Koc value for the micro-lysimeter study was not directly comparable with those for the remaining studies because it was based on linear sorption (nf = 1). Freundlich exponents for the remaining studies were in the range of 0.90-0.94. The Koc value derived by automatic model calibration by group A (37.9 l/kg) agreed

well with that from the laboratory study (39.3 l/kg) whereas the values for automatic and manual calibration by group B were smaller (12.4 and 19.5 l/kg, respectively). Automatic calibration by the two groups resulted in different calibrated parameters (Table 5), but simulated patterns of concentrations were similar (Figure 1). Discrepancies between results from the two groups and between manual and automatic calibration may be caused by several factors, including differences in the calibration of hydrology, the models used to simulate pesticide leaching (PESTRAS vs. PEARL), parameters not included in the calibration, the procedure used to calculate concentrations at the time of sampling and optimisation criteria.

EXTRAPOLATION

The parameters estimated from the lysimeter study should be considered as independent results and should be verified. Koc and DT50 values derived using different approaches were used to simulate the behaviour of compound Y following the last application to three Canadian field sites where environmental conditions differed markedly from those in the lysimeter studies. A comparison was made between (i) the total simulated and measured residues in the field (Figure 2) and (ii) the distribution of residues within the soil profile (Figure 3). The application rate was adjusted in the models in order to match the maximum residue in soil which was observed 1-3 days after application.

The persistence of compound Y in Canadian field studies was over-estimated when laboratory DT50 values were used (Figure 2). The use of DT50 values calibrated against data obtained under outdoor lysimeter conditions resulted in a close fit. Although the DT50 values were almost identical, PEARL predicted faster dissipation than PESTRAS for CAN10 ; this was due to differences in other parameters influencing degradation and in simulated movement of pesticide to depth. Simulated dissipation over winter at CAN11 using PEARL was slower and matched the data better than PESTRAS, because PEARL assumes smaller degradation rates than PESTRAS below 5°C and zero degradation below 0°C. Concentrations of the pesticide within the soil profile (Figure 3) were better simulated when calibrated parameters from dynamic systems were used for modelling compared with laboratory data from static systems.
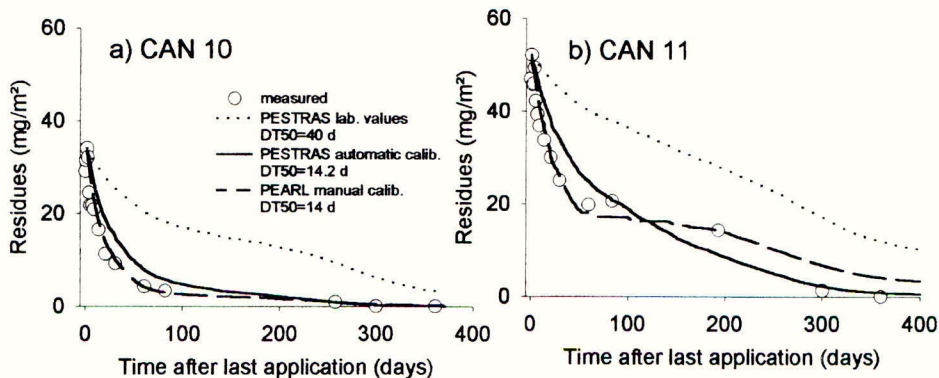

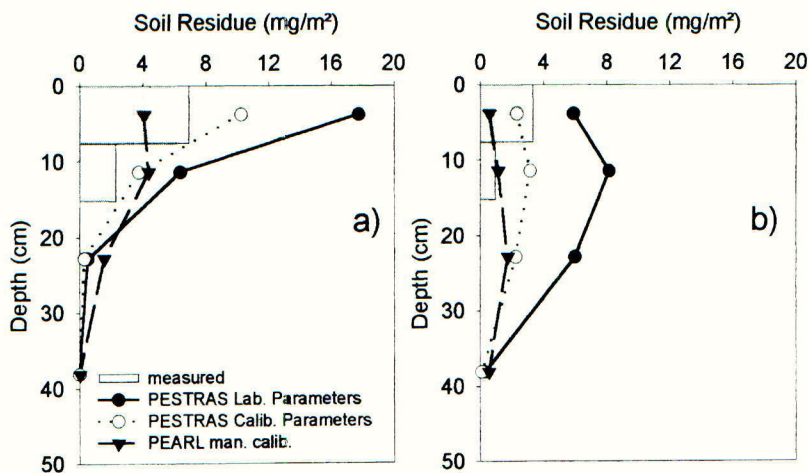Figure 2. Measured and simulated residues of compound Y in the Canadian field studies

Figure 3. Measured and simulated distribution of residues in the CAN10 field study
(a) after 31 days (b) after 61 days

CONCLUSIONS

Degradation parameters derived from experiments under dynamic conditions appear to give better estimates of pesticide behaviour in the field than those from traditional laboratory studies. A significant improvement of the predictive capacity of pesticide fate models can be achieved. Non-uniqueness of parameter sets obtained by calibration should be noted but discussed in the context of the variability of laboratory parameters. The calibrated parameters have to be verified with independent experimental results before they are used for extrapolation to different environmental conditions. The sequence calibration -> verification -> extrapolation should be followed. Possible implications for regulatory experiments and the modelling of pesticide fate should be investigated further.

ACKNOWLEDGEMENTS

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Evaluation of lysimeter experiments in the Netherlands: case studies

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ABSTRACT

The tiered approach in the admission of plant protection products in Europe opens the opportunity to perform higher tier experiments like lysimeter studies, if in the first tier there appears to be a risk of leaching. The interpretation of such studies requires a great deal of expert judgement, which makes a more transparent standardisation method desirable. Simulation models can be used to translate the results of lysimeter studies to other leaching scenarios. However simulated results of lysimeter experiments usually deviate from measured concentrations. This paper gives a suggestion on how to cope with these deviations in the evaluation procedure. A lysimeter study should be computer-simulated as well as possible. The resulting ratio between calculated and simulated leaching, called the simulation error, might be used as a correction for the estimated leaching for other scenarios. Simulation errors however may vary substantially. This variability is used to derive upper confidence limits for the leaching in evaluation scenarios.

INTRODUCTION

The leaching potential of a plant protection product is usually assessed following a tiered approach. Lysimeter experiments enter the assessment when in the first tier it is concluded that there is some risk of leaching. Evaluation of higher tier experiments and their use in taking decisions requires a great deal of expert judgement. To avoid too great an influence of expert judgement in decision making, a transparent standardisation method is required.

A computer simulation model can be used to translate the results of lysimeter studies by comparing measured and computed leaching. A proposal for a standardisation method was done by van de Veen & Boesten (1996), who used the model PESTLA to describe lysimeter studies. Because of the rather large variability in lysimeter experiments, interpretation still required experts. Therefore the search for more transparent interpretation methods continued. In the Netherlands a group of experts from various research institutes developed a guidance for the interpretation of lysimeter experiments (Verschoor *et al.*, 2001). This guidance describes how to convert expert judgement to quantitative rules for evaluation. The lysimeter study should be computer-simulated as well as possible and the result is compared with measured leaching. The resulting ratio between calculated and measured leaching is the so-called simulation error.

Eq. 1

$$SE = \frac{C_{lys}}{M_{lys}}$$

SE = simulation error
C_{lys} = cumulative leaching simulated
M_{lys} = cumulative leaching measured

The simulation error is based on the accumulated leaching, which seems to be a robust parameter in simulation and is also easily obtained from measurements. With the calculated

simulation error it will be possible to extrapolate the results of lysimeter studies to any scenario, for example a vulnerable scenario in the area of intended use. In a deterministic approach the refined estimated concentration can be calculated by:

Eq. 2
$$C_{re} = \frac{C_{target}}{SE}$$

C_{re} = refined estimated concentration (μg/l)
C_{target} = max. concentration in the upper groundwater in a target use scenario (μg/l)

However, reported simulation errors are sometimes rather large (Dressel, 2000). This would mean that a large correction should be made to obtain the refined estimated concentration, which is undesirable. In this paper we show that simulation errors might decrease if full advantage is taken of model options to describe the lysimeter scenario adequately. Furthermore, a proposal for development of the standardisation procedure to fit a probabilistic approach is provided.

METHOD

Existing data for a number of lysimeter experiments from a study by BASF (Dressel, 2000) were reinterpreted with the help of the PEARL model (Tiktak et al., 2000; Leistra et al., 2001). For this purpose original model input (for the leaching model PESTRAS) was adjusted to fit the PEARL input requirements. Several scenario options within the model PEARL were used to refine the predicted leaching of a compound. In the simulation model, PEARL, the user is able to account for pH-dependent sorption and non-equilibrium sorption. Incorporation of these variables in the simulation might reduce the calculated simulation error.

From the ratio between simulated and measured mass fluxes, simulation errors were calculated according to equation 1. The distribution of the simulation errors is used to derive a statistical method to introduce a correction variable for use in registration procedures. In principle only those lysimeters were used with at least one of the input parameters sorption and degradation determined for the specific lysimeter soil. If more than ten DT_{50} and K_{om} values were available from laboratory studies median values were sometimes used.

RESULTS AND DISCUSSION

The cumulative mass flux for all lysimeters was calculated over a period of at least three full years whereas measurements proceeded over a much shorter period of time. The simulations, however indicate that the time span of the measurements was sufficient to measure the cumulative leaching. An example of one of the simulations is shown in Figure 1.

Table 1 summarises the results of the simulations done for 7 lysimeter studies, performed with one compound, and states the calculated simulation errors.
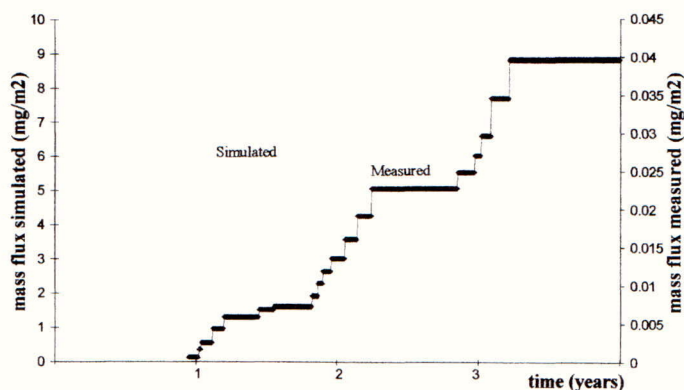
Figure 1. Example of measured and simulated mass fluxes in one lysimeter.

Table 1: Mass fluxes (mg/m^2) of substance at lower boundary and calculated simulation errors for all simulations.

Study	Mass flux measured	Cumulative mass flux at lower boundary for simulation options			Simulation error for simulation options		
		standard	non equi-librium	pH dependent	standard	non equi-librium	PH dependent
1	0.0042	0.36	0.19	0.011	84.75	45.45	2.69
2	0.0156	0.57	0.30	0.098	37.03	19.23	6.27
3	0.0433	0.89	0.46	0.134	20.41	10.64	3.09
4	0.0297	1.84	0.90	0.239	62.50	30.30	8.03
5	0.0463	2.52	1.18	0.284	55.56	25.64	6.13
6	0.038	1.58	0.12	1.84	41.58	3.24	48.4
7	0.0143	0.24	0.016	0.431	16.67	1.09	30.2

Standard calculation

Simulation of the lysimeter scenario with the PEARL model with default options for sorption parameters resulted in calculated simulation errors of 17 to 85. This indicates an overestimation by the model of the total mass of substance leached with these factors. The description of the leaching behaviour by the model seems to be not very accurate.

Effect of non-equilibrium sorption

The PEARL model has an option to account for non-equilibrium sorption (Tiktak *et al.*, 2000; Leistra *et al.*, 2001). Adding non-equilibrium sorption may reduce leaching and therefore reduce overestimation by the model, or in other words decrease the simulation error. For the simulations here the recommended default values for the parameters describing the non-equilibrium sorption process were used.

Using the non-equilibrium sorption option in PEARL requires that also the transformation rate of the compound is adjusted (Boesten, this issue), the transformation rate has to be multiplied with a correction factor. A factor of 1.2 was selected to correct the half-live in the simulations.

From the results (Table 1) we see a decrease in simulation error, compared to the standard simulation. This means a decrease in overestimation of leaching by the model. For the lysimeters 6 and 7 the simulation error is almost 1 which means that measured and simulated results are nearly equal. It should be mentioned that for these two lysimeters no data on sorption and transformation for the lysimeter soil are available. Simulations were thus performed with median value from a large number of laboratory experiments. Therefore the low simulation error calculated might be a coincidence.

Effect of pH dependent sorption.

For substances with a low acid dissociation constant (pK_a value) pH dependent sorption may influence leaching. The substance used on the seven lysimeters discussed has a pK_a of 3.3 and therefore simulating pH-dependent sorption would be appropriate. From the available data, sorption constants of 1000 L/kg for the neutral molecule and 10 L/kg for the anion were derived and used as input to the model in these seven lysimeters. In table 1 the results of simulations using pH dependent sorption are reported. In these calculations only equilibrium sorption is considered.

From the results we see that the simulation error decreases for the lysimeters 1 to 5 compared to initial calculations. For the lysimeters 6 and 7 the simulation error increases compared to calculations for non-equilibrium sorption. Again it should be mentioned that DT_{50} and K_{om} values for these lysimeters were not determined for the lysimeter soil and median values were taken. Overall we can say that simulation errors can decrease if we are able to describe the lysimeter more accurately in a simulation model. The availability of information on a lysimeter study is therefore very important.

Assessment factor

From the results we see that for one compound in different scenarios the simulation error can vary by an order of magnitude. Considering this large variation in simulation errors for one compound a decision based on one simulation error only is quite uncertain. In pesticide registration we don't like to underestimate leaching. Therefore a probabilistic approach, in which an assessment factor based on the variability of the simulation error and the number of experiments, seems to be justified.

The calculation of the refined estimate concentration might be done according to equation 3.
Eq. 3

$$C_{re} = \frac{C_{target}}{F}$$

with

$$F \quad = \overline{SE} - t_{prob} * \sigma / \sqrt{n}$$

$\overline{SE}$ = mean simulation error
n = number of simulation errors
σ = standard deviation of population of simulation errors
t_{prob} = χ^2 probability factor
and the mean and standard deviation obtained from a log-normal fit of distribution of the simulation errors.

Now a confidence level, for example 80%, 90% or 95%, has to be chosen to obtain the assessment factor and the refined concentration estimate.

The results of the seven lysimeters discussed here (compound A) and four more experiments (compounds B and C) (Dressel, 2000) were fitted to a log-normal distribution. Simulation errors of compound B were 17.45, 1.92, 13.3 and for compound C 2.22.

Table 2. Statistical parameters of the simulation error according to a log-normal distribution.

	Standard PEARL	Standard PEARL	Non-eq	pH-dep	PESTRAS
Compounds	A (7), B (3), C (1)	A	A	A	A
Mean	38.55	44.55	24.9	14.51	59.94
Stdev	68.07	26.9	48.16	19.4	83.53
Logstd	1.19	0.56	1.25	1.01	1.04
N	11	7	7	7	7

Here we see that the addition of 4 extra simulation errors to the data set results in a decrease in simulation error.

Example

Suppose that the simulation error of a lysimeter experiment is 38.55. If we want to have 80% confidence that we do not underestimate the leaching, the leaching in the target scenario is not divided by 38.55 (according to eq. 2) as was indicated by the single lysimeter experiment, but by 3.81 (according to eq. 3). Suppose that the concentration calculated for the target scenario was 0.3 µg/l. The refined estimate concentration is then 0.3/3.81 = 0.08 µg/l.

In table 3 the influence of additional experiments and the choice of the confidence level on the assessment factor is summarised. If the number of studies increases the assessment factor will increase and the refined concentration will decrease. The calculated concentration in the example can be read as "there is 80% confidence that the concentration leached is lower than 0.08 µg/l".

Table 3. Value of the assessment factor in dependence of the number of lysimeter experiments and the desired confidence level. (avg. simulation error: 38.55, log standard deviation: 1.19).

Prob.	75%	80%	90%	95%
χ^2 value	0.645	0.845	1.282	1.645
n				
1	6.06	3.81	1.15	0.43
2	10.42	7.50	3.22	1.59
3	13.25	10.13	5.07	2.86
4	15.29	12.11	6.66	4.05
5	16.86	13.69	8.01	5.14

It must be emphasised that these calculations are based on 11 separate lysimeter runs only. Consequently the standard deviation is quite large, resulting in relatively large safety margins.

The safety margin, $t_{prob} * \sigma / \sqrt{n}$, can be decreased by:

1. extension of the database containing simulation errors (which decreases σ),
2. providing more lysimeter experiments for the substance of concern (n)
3. choosing a lower confidence level (χ^2).

CONCLUSIONS AND RECOMMENDATIONS

Interpretation of higher tier experiments reveals that models, which are used today in pesticide registration evaluation, are not capable of reproducing exactly the observed leaching levels. When taking advantage of more advanced options of these models, it is possible to reduce deviations. This was demonstrated for a number of studies, using the PEARL model. For the risk assessment reasonable certainty is required that the substance is safe with respect to leaching. Therefore a method is developed to derive assessment factors based on observed simulation errors and basic probabilistic theory; the value of the assessment factor being dependent on the desired confidence level and the number of higher tier experiments for the specific compound. Based on the uncertainty in the simulation error, the assessment factor is usually lower than the simulation error.

The method proposed here was illustrated using 11 lysimeter studies, with only three different substances. We recommend that a larger database is established, covering more compounds. This would supply more insight in the applicability of this method.

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