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Sensitivity analyses for leaching models used for pesticide registration in Europe

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MAFF project PL0532
SSLRC project JF3741E

SSLRC

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by

Igor G. Dubus, Colin D. Brown & Sabine Beulke

Final report
September 2000

MAFF Project PL0532
SSLRC Contract No. JF 3741E

Soil Survey and Land Research Centre
Cranfield University, Silsoe, Beds MK45 4DT, UK
Tel: 01525 863000 Fax 01525 863253
E-mail: soil.survey@cranfield.ac.uk Web: http://www.cranfield.ac.uk/sslrc/

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Foreword

In 1998, the Ministry of Agriculture, Fisheries and Food (MAFF) commissioned SSLRC to undertake sensitivity analyses for the leaching models used for pesticide registration in Europe. This document provides a description of the methods which were adopted for these investigations, a presentation of results obtained and implications of the findings for modelling activities and submission of modelling studies for pesticide registration. More details on the methods and results are presented in a separate document which gathers appendices.

The preferred reference to this report is as follows:

DUBUS I.G., BROWN C.D. & BEULKE S. (2000). Sensitivity analyses for leaching models used for pesticide registration in Europe. SSLRC report for MAFF PL0532, Silsoe, Beds., UK, 85p.

The two other documents produced within the scope of this project are referenced as follows:

DUBUS I.G., BROWN C.D. & BEULKE S. (2000). Sensitivity analyses for leaching models used for pesticide registration in Europe - Appendices. SSLRC report for MAFF PL0532, Silsoe, Beds., UK, 238p.

DUBUS I.G., BROWN C.D. & BEULKE S. (2000). Sensitivity analyses for leaching models used for pesticide registration in Europe - A quick reference guide. SSLRC report for MAFF PL0532, Silsoe, Beds., UK, 82p.

Executive summary

Although pesticide leaching models have played an increasing role in the registration of pesticides in Europe, little is known about which input parameters most influence model predictions. This information is crucial for quality modelling and for an effective assessment of modelling studies which estimate the risk for a pesticide to impact on the environment.

Sensitivity analyses were carried out for the latest versions of the four primary leaching models used for pesticide registration in Europe (PELMO 3.00, PRZM 3.14, PESTLA 3.4 and MACRO 4.1). Sensitivity of the models was investigated using two investigation methods (one-at-a-time sensitivity analysis and Monte Carlo sensitivity analysis) and four scenarios describing the leaching of two pesticides (Pesticide “L”, Koc 20 ml/g, laboratory DT50 value 20 days; Pesticide “T”, Koc 100 ml/g, laboratory DT50 value 100 days) in two soils (a sandy loam of the Wick series and a more structured clay loam of the Hodnet series). The influence of the variation of a large number of input parameters on the prediction of *percolation volumes* and *total pesticide losses* was investigated. Input parameters were varied within bounds defined by their uncertainty.

The magnitude of the sensitivity of the models was found to be dependent on the model output considered. Predictions of *water percolation* were only marginally affected by changes in input parameters considered in this project. The major driver of percolation predictions is therefore the meteorological data, especially rainfall measurements and potential evapotranspiration data. In contrast to percolation, predictions of *pesticide losses* were dependent on a large number of parameters and to a much greater extent. The ranking of input parameters according to their influence on the prediction of pesticide losses was affected by the initial scenario considered. In most model-scenario combinations considered in this study, parameters which had the largest influence on pesticide predictions were those related to <u>sorption</u> (Freundlich coefficient and exponent) and <u>degradation</u> (either degradation rates or DT50 values, QTEN value). A large influence of <u>soil</u> parameters (field capacity, soil moisture content at the beginning of the simulation period and bulk density) was also noted in a small number of specific scenarios for all models. For the dual porosity model MACRO, the influence of sorption and degradation parameters was surpassed by the influence of soil parameters specific to the definition of the boundary between micropores and macropores for one of the two scenarios involving the more structured clay loam.

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Large sensitivities were identified for all four models and model predictions for pesticide losses should therefore be considered as uncertain. Uncertainty is indirectly taken into account at lower tiers of the environmental risk assessment for pesticides by the use of uncertainty factors (*e.g.* in the Toxicity Exposure Ratio approach). At higher tiers, conditions closer to reality are considered and uncertainty factors are reduced or removed. Given the sensitivities reported in this study, it is appropriate that the uncertainty in modelling predictions is taken into account at higher tiers. Results from this study should be considered a starting point to: i) investigate the uncertainty in modelling predictions resulting from uncertainties in model input, and ii) perform probabilistic modelling (*i.e.* include uncertainty considerations in the predictions that are made). The information should also be used when performing model calibrations against experimental data.

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1. INTRODUCTION

Mathematical modelling has been increasingly used in the last two decades to assess the fate of pesticides in the environment and the potential for contamination of surface waters and groundwater. So far, modelling developments have mainly concentrated on the prediction of pesticide losses by leaching (*i.e.* the estimation of the presence of pesticides in the water percolating out of the soil profile). Mathematical modelling has been given a prominent role in the fate and behaviour section of the registration process of plant protection products in Europe following the publication of the EU directive 91/414. According to this document, the environmental risk assessment for pesticides is based on a tiered approach where first assessments are based on simplified assumptions and further investigations of increasing complexity are triggered by the failure to meet threshold criteria. The FOCUS working group on leaching scenarios has recommended the use of four leaching models for pesticide registration (*i.e.* PELMO, PESTLA, PRZM and MACRO). Although these four models are used routinely in the preparation of modelling submissions for registration, little is known about the influence of variation of model input on model predictions (*i.e.* the sensitivity of the models).

The end-product of a sensitivity analysis is traditionally a list of input parameters classified by their influence on selected model predictions. Such information is vital for the overall community of model developers, model users and regulators working on leaching of pesticides in soils. It helps model developers to identify input parameters that have little or no influence on model output and therefore helps them to identify subroutines which could be simplified or deleted. It is also a good way to identify coding errors. A list of the most influential parameters will greatly assist model users. They can concentrate their time and financial resources on selection of the most sensitive parameters and identify the parameters that should be modified first when performing a model calibration. This information also benefits regulators evaluating modelling submissions in highlighting the parameters for which adequate justification in the choice of values is needed and in helping them to focus on the attribution of values to the most important parameters. Finally, results from a sensitivity analysis are useful for identifying research required for strengthening the knowledge base in order to reduce the uncertainty in model predictions.

In this project, we performed sensitivity analyses for the latest versions of the four leaching models used for pesticide registration in the EU (MACRO 4.1, PELMO 3.00, PRZM 3.14β and PESTLA 3.4). Two different investigation methods were used and compared (*i.e.* one-at-a-time and Monte Carlo based sensitivity analyses). Since it is known that results from sensitivity analyses can be dependent on the scenario considered, four different scenarios resulting from the simulation of the fate of two pesticides in two different soils were considered. Sensitivity was investigated with regard to predictions for percolation volumes and pesticide losses via leaching. This document reports on the methodology that was followed and presents the results obtained for each model. Implications for modelling activities and submission of modelling studies to regulatory authorities are put forward. More detailed information on the approach and results is available as appendices in a separate document.

2. MATERIAL AND METHODS

2.1 CASE STUDIES

It has been shown that results of sensitivity analyses are dependent on the base-case scenarios that have been selected (Ferreira *et al.*, 1995). With regard to pesticide fate models, it is not expected that the most sensitive parameters for leaching models will be the same in a sandy and in a clay soil, for instance. Similarly, models may not show the same sensitivity for different molecules. It was therefore decided to conduct the sensitivity analysis on a total of four different scenarios to cover a range of environmental situations. Sensitivity was investigated for the leaching of two pesticides with contrasting properties in a sandy loam and a clay loam soil. A single weather dataset was used for all scenarios.

2.1.1 Weather data

Weather data were selected from long-term measurements from the Wrest Park weather station (Silsoe, Bedfordshire, UK). The year 1979 was chosen from a 30-year dataset as being wetter than average (700.4 mm of rainfall compared to a long-term mean of 575 mm, 97^{th} percentile for the period 1965-1996 in Silsoe), and as being particularly wet during the winter and spring periods (Table 1). This choice was made to ensure that the weather scenario would be relevant to a large portion of the country and Europe, and that the pesticides which were chosen would leach to at least 1-m depth.

Potential evapotranspiration (PET) was calculated outside the various models using the Penman-Monteith formula (FAO, 1991) and detailed meteorological information. Monthly summaries for the weather dataset are provided in Table 1.

The data were repeated to enable a maximum simulation of 10 years. The reason for repeating a year rather than taking real meteorological data for 10 years is that models were run for the minimum amount of time that encompassed the full leaching breakthrough. Having the same weather information between years meant that the comparison between modelling scenarios with different duration was still meaningful.

	Rainfall mm	Mean air temperature °C	Mean air minimum temp. °C	Mean air maximum temp. °C	PET mm	Sunshine hours
January	51.4	-0.8	-4.2	2.5	7.5	57.5
February	36.8	0.9	-1.4	3.2	12.0	55.0
March	101.6	4.7	1.4	8.1	34.1	99.6
April	73.8	7.7	3.8	11.6	55.2	116.5
May	72.0	10.7	6.0	15.3	86.6	196.7
June	23.0	13.8	9.2	18.3	89.0	164.0
July	12.0	16.1	10.9	21.4	103.4	181.5
August	107.8	15.5	10.7	20.3	85.0	175.9
September	12.3	13.5	8.3	18.7	61.8	170.5
October	61.4	10.8	6.4	15.2	28.5	125.3
November	40.8	6.4	3.0	9.8	14.7	67.4
December	107.5	5.7	3.1	8.4	14.6	58.2
Total	700.4	8.7	4.8	12.7	592.3	1468.1

Table 1. Monthly summary of meteorological data for the year 1979 in Silsoe, Beds., UK

2.1.2 Soil and cropping data

Soils from the Wick (sandy loam) and Hodnet (clay loam) series were selected to reflect contrasting conditions with regard to the transfer of water and solutes. These two soils are being used in an on-going MAFF funded lysimeter study (PL0523, Lysimeter study to investigate the effect of rainfall patterns on pesticide leaching and the viability of stochastic modelling approaches for risk quantification) and detailed profile information and soil properties were available.

Soils of the Wick series are deep, uniformly coarse textured, free draining sandy loams formed on loose, sandy or sandy gravelly glacial, fluvoglacial or river terrace deposits. They have low water retention and, under arable cultivation, low organic matter contents. The soils normally overlie local aquifers or groundwater bodies at between 2 and 10 metres from the surface. Wick soils were selected for this study because they are extensively used for arable cropping and have a high soil leaching potential. According to the Environment Agency's groundwater vulnerability classification (NRA, 1992), they are grouped with class H2 soils which readily transmit a wide range of pollutants because of their rapid drainage and low attenuation potential. Wick soils and their hydrological equivalents (HOST class 5; Boorman *et al.*, 1995) are widely distributed throughout England and Wales (765,448 ha, 7.3% of agricultural land).

Soils of the Hodnet series are deep, fine loamy, reddish soils formed on interbedded reddish sandstones and mudstones. They have slowly permeable horizons in the subsoil which restrict the downwards movement of water and these soils are occasionally waterlogged (wetness class II or III). Hodnet soils belong to HOST class 18 which occupies 861,553 ha in England and Wales (8.3% of agricultural land).

Tables 2 and 3 present selected physico-chemical characteristics and water retention data for the two soils. Soil profiles were adjusted to 1-m depth to enable a sound comparison between model results from the different scenarios.

	Wick				Hodnet			
	0-20 cm	20-50 cm	50-75 cm	75-100 cm	0-33 cm	33-60 cm	60-80 cm	80-100 cm
Organic carbon (%)	1.70	0.80	0.30	0.20	1.15	0.48	0.40	0.30
Sand (%)	57	70	73	77	33	42	29	26
Silt (%)	33	20	16	9	48	42	48	55
Clay (%)	10	10	11	14	19	16	23	19
Texture[a]	SL	SL	SL	SL	CL	ZCL	CL	CL
Bulk density	1.35	1.45	1.41	1.53	1.39	1.62	1.55	1.48
pH H_2O	6.5	7.0	7.0	6.9	6.7	6.8	6.8	6.8

[a] SL: sandy loam, CL: clay loam, ZCL: silty clay loam

Table 2. Selected physicochemical properties for the Wick and Hodnet soils

	Wick				Hodnet			
	0-20 cm	20-50 cm	50-75 cm	75-100 cm	0-33 cm	33-60 cm	60-80 cm	80-100 cm
W_{0kPa} (% vol)	46.6	39.6	39.0	34.3	46.8	38.8	41.5	44.0
W_{5kPa} (% vol)	27.8	19.1	14.7	19.2	34.9	30.8	32.2	35.8
W_{10kPa} (% vol)	24.1	17.0	11.7	16.4	33.7	29.9	31.4	35.0
W_{40kPa} (% vol)	19.7	14.2	8.7	13.4	31.2	26.7	28.9	31.8
W_{200kPa} (% vol)	15.1	10.8	6.0	9.8	25.1	24.2	24.5	26.6
$W_{1500kPa}$ (% vol)	10.5	7.9	4.4	7.7	16.8	17.9	19.9	20.1

Table 3. Water retention data for the Wick and Hodnet soils (soil water content for a given pressure)

The simulated crop was winter wheat in each year and this was considered to emerge on 12 October and to be harvested on 7 August the next year (crop maturation was considered to occur on 24 June). These cropping dates are typical of wheat cultivation in the UK (Hough, 1990).

2.1.3 Pesticide and application data

Two hypothetical molecules with different sorption and degradation properties were considered. The properties of the two pesticides are presented in Table 4. The first compound (Pesticide L) has a Koc of 20 ml g^{-1}, a field DT50 of 20 days and is slightly volatile. The second molecule (Pesticide T) is non-volatile and has larger Koc and field DT50 (100 ml g^{-1} and 60 days, respectively). Both molecules are classified as ‘Leachers’ according to the GUS classification (Gustafson, 1989) and are therefore likely to move out of the soil profile in some circumstances. These basic properties were used for all four scenarios for the four models.

The two pesticides were considered to be applied on 1 November of the first year only at an application rate of 2.0 kg a.s. ha^{-1}. No correction was made to account for interception of the spraying solution by the crop.

	Pesticide L	Pesticide T
Sorption		
Koc (ml g^{-1})	20.0	100.0
Kom (ml g^{-1})	11.6	58.1
Degradation		
DT50 at 8°C (days)	20	60
DT50 at 20°C (days)	7.8	23.3
k_{deg} at 20°C (day^{-1})	0.0893	0.0298
Volatility		
H (J mol^{-1}) at 20°C	1.2×10^{-3}	2.4×10^{-7}
H' (dimensionless) at 20°C	5.0×10^{-7}	1.0×10^{-10}

Table 4. Sorption, degradation and volatility characteristics of the two hypothetical pesticides

2.1.4 Modelling strategy

The fate of the two molecules in the two contrasting soils was predicted using PELMO 3.00 (July 1998), PESTLA 3.4 (September 1999), PRZM 3.14 in its β version (December 1999) and MACRO 4.1 (July 1998). The sensitivity of the four models was assessed using the predictions for percolation ("percolation" in MACRO and PESTLA, "recharge" in PELMO and PRZM) and for total pesticide losses in leachate over the running period. No calibration against measured data was carried out. Models were run for the minimum amount of time that allowed full leaching breakthrough to occur.

The four scenarios were referred to using a combination of three letters. The first letter designates the model (M=MACRO, O=PELMO, A=PESTLA, Z=PRZM), the second letter designates the pesticide (L or T) and the third letter designates the soil (W=Wick series, H=Hodnet series). For instance, MLW refers to the prediction of the fate of pesticide L in the Wick soil by the MACRO model.

2.1.4.1 MACRO

Preliminary tests on the four scenarios selected for investigation of sensitivity revealed that the minimum number of years needed to include all pesticide losses in percolation was four years except for the scenario "Pesticide T on Wick" for which six years were required. Comparisons between all four scenarios remained possible because predicted annual recharge is constant throughout the simulation period except for the first year and cumulative loss is used. A total of 43 “primary” parameters was considered for variation (Table 5). Where parameters were depth-dependent, input values for the subsoil were modified at the same time as parameters for the topsoil by linking them using coefficients derived from the base scenarios (*e.g.* when the sorption coefficient was modified by 10% in the topsoil, the values for the subsoil were varied by the same percentage). In the end, a total of 99 input parameters were varied (43 primary parameters + 56 linked parameters). Degradation rates were varied with depth according to the equation implemented in MACRO_DB (Jarvis *et al.*, 1997). Initial moisture contents at the start of the simulation were set to field capacity. An example input file (scenario MLW) is provided in Appendix 1.

	Parameter	Brief description	Links between topsoil and subsoil parameters
1	ANNAMP	Temperature annual amplitude	
2	ANNTAV	Average annual temperature	
3	ASCALE	Effective diffusion pathlength	✓
4	BETA	Root adaptability factor	
5	CANCAP	Canopy Interception Capacity	
6	CANDEG	Canopy degradation rate	
7	CFORM	Form factor	
8	CRITAIR	Critical soil air content for root water uptake	
9	CTEN	Boundary soil water tension	✓
10	DEG	Degradation rates	✓
11	DFORM	Form factor	
12	DIFF	Diffusion coefficient in water	
13	DV	Dispersivity	
14	EXPB	Exponent moisture relation	
15	FEXT	Canopy wash-off coefficient	
16	FRACMAC	Fraction sorption sites in macropores	
17	FREUND	Freundlich exponent	
18	FSTAR	Solute concentration factor	
19	GAMMA	Bulk density	✓
20	KSATMIN	Saturated hydraulic conductivity	✓
21	KSM	Boundary hydraulic conductivity	✓
22	LAIHAR	Leaf Area Index at harvest	
23	LAIMAX	Maximum Leaf Area Index	
24	LAIMIN	Leaf Area Index at zdatemin	
25	RINTEN	Rainfall intensity	
26	ROOTINIT	Root Depth at zdatemin	
27	ROOTMAX	Maximum root depth	
28	RPIN	Root distribution	
29	TEMPINI	Initial soil temperature	✓
30	THETAINI	Initial soil moisture	✓
31	TPORV	Saturated water content	✓
32	TRESP	Exponent temperature response	
33	WATEN	Critical water tension for root water uptake	
34	WILT	Wilting point	✓
35	XMPOR	Boundary soil water content	✓
36	ZALP	Correction factor for wet canopy evaporation	
37	ZFINT	Fraction of irrigation intercepted by canopy	
38	ZHMIN	Crop height at zdatemin	
39	ZKD	Sorption coefficient	✓
40	ZLAMB	Pore size distribution index	✓
41	ZM	Tortuosity factor micropores	✓
42	ZMIX	Mixing depth	
43	ZN	Pore size distribution factor macropores	✓

Table 5. List of MACRO parameters which were included in the sensitivity analysis

2.1.4.2 PELMO

Preliminary tests conducted for the four scenarios revealed that the running time sufficient to achieve complete leaching of the two pesticides was four years for the OLW scenario, nine years for the OTW scenario, seven years for the OLH scenario and ten years for the OTH scenario. These leaching times are significantly larger than those for MACRO.

Four options are proposed for the flag regulating the introduction of evapotranspiration in PELMO (1. calculation of potential evapotranspiration (PET) using temperature only; 2. use of measured pan evaporation data; 3. calculation of PET using the Haude formula; 4. own data). Since PET was calculated outside the model using the Penman-Monteith equation, PET data were directly fed into the model using option 4 and runs were carried out using this procedure. Although this is not specified in the PELMO user's manual, option 4 corresponds to a situation where crop-specific evapotranspiration data have been measured in the field (hence results obtained when running PELMO with option 4 and option 2 with a pan factor of 1 are different). It is desirable that modellers are made aware of the detailed data requirements of option 4 since this is not specified in the user's manual of PELMO and this might lead to inaccuracies if PET data estimated by standard equations are fed into the model using option 4. Checking tests were carried out after the main runs and showed that the use of option 4 for the evaporation flag in this study resulted in the lack of sensitivity of the prediction of recharge by PELMO to the parameters ANET (minimum depth for evaporation) and AMXD (maximum active root depth). This is because PELMO assumes that water extracted by evaporation is taken within a constant profile depth when option 4 is selected.

PELMO offers the possibility to simulate both pesticide losses induced by run-off and the effect on leaching of an increase in sorption with time. These features were not used in this study because it was decided to maintain consistency of approach for all four leaching models. Sorption coefficients and degradation coefficients were introduced directly into the model. Degradation rates were varied with depth using the same factors as used for MACRO.

Table 6 presents the 18 “primary” parameters within PELMO which were considered for investigation. Adding the parameters that were linked to the primary variables, 44 parameters were varied in total. Examples of input files (scenario OLW) are provided in Appendices 59 and 60.

Water content at the beginning of the simulation (WC) was set to field capacity (FC).

	Parameter	Brief description	Links between topsoil and subsoil parameters
1	ANET	Depth to which ET is computed	
2	CINT	Average annual temperature	
3	AMXD	Maximum active rooting depth	
4	COVM	Maximum areal coverage	
5	UPTK	Plant uptake efficiency factor	
6	BUD	Bulk density	✓
7	WC	Initial soil water content	✓
8	FC	Field capacity	✓
9	WP	Wilting point	✓
10	PDRA	Plant decay rate	
11	FEXT	Foliar extraction coefficient	
12	HENR	Henry's constant	
13	DEGR	Degradation rate	✓
14	QTEN	Increase given a temperature increase of 10°C	
15	ASM	Absolute soil moisture	
16	MEXP	Exponent for moisture correction	
17	KF	Freundlich coefficient	✓
18	NF	Freundlich exponent	✓

Table 6. List of PELMO parameters which were included in the sensitivity analysis

2.1.4.3 PRZM

The version of PRZM which was used was that produced for the integration of the FOCUS scenarios (version 3.14β, "FOCUS release"). However, the executable WINPRZM was used as a standalone program outside the Windows FGRAT shell. This particular version was used because version 3.12 does not include descriptions of either sorption by the Freundlich equation or the influence of soil moisture and temperature on degradation. The use of the upgraded version ensured that all models considered in this project used had more or less the same capabilities with regard to the description of sorption and degradation. It was decided to run the PRZM model for 10 years, irrespective of the time required for total loss of the pesticides by leaching because the running time for 10 years is insignificant compared to that for other models. Examination of the initial runs confirmed that a running time of 10 years allowed total leaching of both pesticides in the two soils.

PRZM offers the possibility of simulating volatilisation, an increase in sorption with time and of describing degradation using a bi-phasic equation, but corresponding subroutines were turned off. The Kd values for the parameters related to sorption were directly input into the files (*i.e.* the Koc option was not used). Degradation rates were varied with depth using the same factors as for MACRO. Water content at the beginning of the simulation was set to the value for field capacity.

A list of all PRZM parameters considered for variation in this exercise is presented in Table 7. A total of 40 parameters were included in the sensitivity analysis (*i.e.* 22 primary parameters and 18 subsoil parameters for which variation was linked to that for topsoil parameters). An example input file (scenario ZLW) is provided in Appendix 116.

	Parameter	Brief description	Links between topsoil and subsoil parameters
1	ANET	Minimum depth for extraction of evaporation	
2	CINT	Maximum interception storage	
3	AMXD	Maximum rooting depth	
4	COVM	Maximum areal coverage of canopy	
5	HTMA	Maximum canopy height	
6	UPTK	Plant uptake factor	
7	PLDK	Pesticide decay rate on canopy	
8	FEXT	Foliar extraction coefficient	
9	NF	Freundlich exponent	
10	A	Albedo	
11	EM	Emmissivity	
12	T	Average monthly temp at BB	
13	QTEN	qten	
14	MEXP	Moisture exponent for degradation	
15	ASM	Reference moisture for degradation	
16	BD	Bulk density	✓
17	FC	Field Capacity	✓
18	DEG	Degradation rate	✓
19	WP	Wilting point	✓
20	OC	Organic carbon content	✓
21	KD	Freundlich coefficient	✓
22	TINI	Initial temp of the horizon	

Table 7. List of PRZM parameters which were included in the sensitivity analysis

2.1.4.4 PESTLA

Although preliminary tests revealed that six years were necessary to achieve complete leaching of the two pesticides in the soils considered, SWAP/PESTLA were run for a total of 10 years as this enabled an easier processing of model output. A total of 34 primary input parameters were considered for variation (Table 8). Where parameters were depth-dependent, parameters for the subsoil were modified at the same time as those for the topsoil by linking them using coefficients derived from the base-case scenarios. In the end, a total of 142 values for input parameters was modified (34 primary input parameters + 108 tied parameters).

Sorption was described using the Kom concept and sorption coefficients were therefore varied with depth according to the organic matter content. Factors for the modification of degradation with depth were similar to those used for MACRO and were kept to their nominal values. Example of input files (scenario ALW) are provided in Appendices 174-181.

	Parameter	**Brief description**	**SWAP (S) / PESTLA (P)**	**Links between topsoil and subsoil parameters**
1	G1	Residual moisture content	S	✓
2	G2	Saturated moisture content	S	✓
3	G3	Saturated hydraulic conductivity	S	✓
4	G4	Alpha main drying curve	S	✓
5	G6	Parameter n	S	✓
6	COFR	Soil evaporation coefficient of Blak and Boesten or Boesten/Stroosnijder	S	
7	RSIG	Minimum rainfall to reset models	S	
8	PSA	sand content	S	✓
9	PSI	silt content	S	✓
10	PCL	clay content	S	✓
11	ORG	organic matter content	S, P	✓
12	RDS	maximum rooting depth allowed by soil profile	S	
13	HI	initial pressure heads	S	✓
14	TEMI	initial soil temperatures	S	✓
15	IF1	Extinction coefficient for diffuse visible light	S	
16	IR1	Extinction coefficient for direct visible light	S	
17	GCTB	Maximum leaf area index	S	
18	CFTB	Crop factor	S	
19	RDTB	maximum rooting depth	S	
20	RDD	Root density distribution	S	
21	BD	Bulk density	P	✓
22	LEDS	Lengths of dispersion in liquid phase	P	✓
23	THAI	Thickness of the stagnant air layer at soil surface	P	
24	SUWA	Coefficient of diffusion in water	P	
25	SUAI	Coefficient of diffusion in air	P	
26	ENSL	Molar enthalpy of the dissolution process	P	
27	SAVP	Saturated vapour pressure	P	
28	ENVP	Molar enthalpy of the vaporisation process	P	
29	CFUP	Coefficient of uptake by plants	P	
30	DEG	Half-life	P	
31	EGCV	Molar activation energy of degradation	P	
32	CFLI	Coefficient describing the relationship between the conversion rate and the volume fraction of liquid	P	
33	KOM	Kom	P	
34	FREU	Freundlich exponent	P	

Table 8. List of PESTLA parameters which were included in the sensitivity analysis

2.2 COMBINATION OF *SENSAN* AND PESTICIDE FATE MODELS

2.2.1 The *SENSAN* package

SENSAN (February 1997 version) is a software package running in the DOS environment which facilitates the sensitivity analysis process by allowing a modeller to automate the task of adjusting certain model inputs, running the model, reading the outputs of interest, recording their values (and the whole output file if necessary) and then commencing the whole cycle again. SENSAN reads user-prepared parameter values and writes specified model output values to files which can easily be imported/exported to a spreadsheet for further post-processing. SENSAN communicates with the model exclusively through input and output files and is therefore model-independent and does not require any recoding of the different models. SENSAN is based on the same parameter recognition techniques implemented in the inverse modelling package PEST (Doherty *et al.*, 1994).

SENSAN uses *template files* (*.tpl) to modify the selected parameters in the input files and records selected model outputs using *instruction files* (*.ins). Values to be assigned to input parameters are stored in a *variation file* (*.var) and ouput values are gathered in *run record files (*.sss)*. The whole parameterisation of SENSAN is implemented in the *control file* (*.sns).

2.2.2 Establishment of a relationship between SENSAN and pesticide fate models

SENSAN was linked to the four pesticide fate models through their input and output files and via batch files. Selected outputs were recorded after post-processing for the four models. Flow charts describing the combination of SENSAN with the four models are provided in Appendices 2, 61, 117 and 182. Model output files were documented and archived after each run to enable possible further use of this large amount of data in the future.

The outputs that were used to reflect the sensitivity of the models were the cumulative percolation (‘recharge’ for some models) [in mm] and the cumulative loss of pesticide by this pathway [in g/ha] over a number of years. These outputs were not produced directly by the four models and they were therefore computed automatically from other model outputs.

For MACRO, the binary output file produced by the model was post-processed automatically by a batch file which generated a file with the values of the cumulative percolation (MACRO parameter 'TFLOWOUT') and cumulative solute leaching (MACRO parameter 'TSOUT'). The SENSAN instruction file then read the last values of the file. Cumulative solute leaching was converted from mg/m^2 to g/ha.

For PELMO, cumulative recharge was calculated from the annual values of 'recharge below soil core' (in cm of water) which can be found in the 'wasser.plm' output file. Similarly, cumulative pesticide losses were computed from values of 'pesticide leached below core' (given in kg/ha) in the 'chem.plm' output file for each year of the simulation period.

For PRZM, cumulative recharge was taken from the annual values for the 'leaching output' for the bottom layer of the profile (in cm of water). As for PELMO, cumulative pesticide losses were computed from annual values for 'pesticide leached below core depth' (given in kg/ha).

For PESTLA, annual percolation was extracted from the file "bawafc.out" (PRBT=water percolated annually through the bottom of the system, in mm). Pesticide losses were computed from the cumulative loss per area out of the bottom of the system (in kg/ha) from the file "leacos1.out". Cumulative pesticide losses were converted from kg/ha to g/ha.

2.3 ONE-AT-A-TIME SENSITIVITY ANALYSIS

2.3.1 Approach

One-at-a-time sensitivity analysis is the simplest approach of its kind. The general framework is to repeatedly vary one parameter at a time while holding the others fixed. It is easy to conduct and produces results that can be readily presented in a graphical form. A sensitivity coefficient is the ratio of the change in output to the change in input while all other parameters remain constant (Krieger *et al.*, 1977). The model output when all parameters are kept constant at their nominal values is defined as the 'base case'. The main disadvantage of this approach is that the conclusions that are derived are specific to the base-case scenario. Furthermore, sensitivity is assessed on individual parameters without regard to the combined variability resulting from considering all input parameters simultaneously.

The parameters can be changed either by a constant percentage (local sensitivity analysis) or by a factor of their standard deviation (this approach takes into account parameter variability). In this study, it was considered that larger benefits would be gained by varying the parameters within a range defined by their uncertainty. Hence, the present study can be considered as a first-step uncertainty analysis where variation of the parameters was attributed by expert knowledge.

2.3.2 Derivation of variation range of input parameters

Variation ranges were attributed to input parameters using expert judgement only. The derivation of variation ranges from literature review or experimental data was outside the scope of this study. Range of variation for each parameter was discussed between three experienced modellers until consensus was achieved for all parameters.
Parameters which are traditionally determined through experimental measurements were varied symmetrically (*i.e.* same variation for increase and decrease of the parameter). Parameters related to sorption and degradation were considered as relatively uncertain. For most of them, it was considered that a reasonable range of variation was obtained by multiplying and dividing the average value by a factor of 2. Parameters that cannot be determined experimentally were varied according to expert judgement. Where appropriate, model authors were contacted to discuss particular parameter variations. Finally, parameters that are highly uncertain were varied by a factor of 10 or more. Attention was paid to vary the parameters in the same way between models to enable a direct comparison of results.

2.2.3 Treatment of modelling results

Assume that an input parameter I has been varied from its base-case value I_{BC} and that in response to this variation, the model has produced an output value O that is different from the base-case value for the output O_{BC}.

The variation in the input parameter can be expressed as:

$$\text{Input variation in \%} = (I-I_{BC})/I_{BC}*100$$

Similarly, the variation in the output parameter can be expressed as:

$$\text{Output variation in \%} = (O-O_{BC})/O_{BC}*100$$

The plotting of the output variation vs. the input variation provides a graphical means to assess the sensitivity of the model to input parameters. The closer the curve to the Y axis (the larger the slope of the line linking the origin and a particular point), the more sensitive to this parameter the model is. In the same way, the closer the curve to the X axis (the smaller the slope of the line linking the origin and a particular point), the less sensitive to this parameter the model is.

Numerically, a *ratio of variation* (ROV) can be defined as follows:

$$ROV = \text{Output variation} / \text{Input variation}$$

Or, $$ROV = ([O-O_{BC}]/[I-I_{BC}]) * (I_{BC}/O_{BC})$$

This variation can be either positive or negative. It takes negative values if a decrease in an input parameter results in an increase in the output value or if an increase in an input parameter results in a decrease in the output value. The sign of the ratio is not critical when the aim is to classify the input parameters by their influence on model output. Hence, the absolute value of ROV (|ROV|) was considered for classification purposes.

It was decided to represent the influence of a particular input parameter by the maximum absolute ratio of variation (MAROV), *i.e.* maximum slope of the lines linking the origin to data points in the graph of output variation vs. input variation.

$$MAROV = Max_i\ |ROV|, \qquad i = 1 \text{ to } r,$$

where r is the number of model runs carried out for a particular parameter.

The larger the MAROV index, the more influence a parameter has on model output. A MAROV of 1 means that a variation in the model input of *x*% will result at maximum in the same variation in the model output (*x*%). If MAROV equals 10, the disturbance of a model input will be propagated through the model and amplified to result in a maximum variation of the output by 10 times more. A conversion table for MAROV is presented in Table 9.

MAROV value	The variation in the input by	results in a variation in the output by	which represents a multiplication factor for the output of
0.01	10% (*e.g.* 100 to 110)	0.1% (*e.g.* 100 to 100.1)	1.001
0.25	10% (*e.g.* 100 to 110)	2.5 % (*e.g.* 100 to 102.5)	1.025
0.5	10% (*e.g.* 100 to 110)	5 % (*e.g.* 100 to 105)	1.05
1	10% (*e.g.* 100 to 110)	10 % (*e.g.* 100 to 110)	1.1
2	10% (*e.g.* 100 to 110)	20 % (*e.g.* 100 to 120)	1.2
5	10% (*e.g.* 100 to 110)	50 % (*e.g.* 100 to 150)	1.5
10	10% (*e.g.* 100 to 110)	100 % (*e.g.* 100 to 200)	2
90	10% (*e.g.* 100 to 110)	900 % (*e.g.* 100 to 1000)	10
990	10% (*e.g.* 100 to 110)	9900 % (*e.g.* 100 to 10000)	100
9990	10% (*e.g.* 100 to 110)	99900 % (*e.g.* 100 to 100000)	1000

Table 9. Variations in the output for different MAROV values

Since MAROV values can be highly dependent on a single data point, it is very important not to consider the MAROV values *per se*. Instead, the most important feature is the ranking of parameters. Additionally, the information is presented by classifying the parameters into sensitivity classes (Table 10). Although this classification is rather subjective, it enables an easy presentation and understanding of the results (Figure 1).

The reason for using three different ways of presenting the results (charts presenting variation in output vs. variation in input, MAROV values and parameter ranking) is that data presentation format has been shown to influence perceived model sensitivity (Ferreira *et al.*, 1995). The presentation of the same data by different representations is likely to benefit the use of information generated by sensitivity analysis.

MAROV values	Classification of parameters
>10	Extremely sensitive
1-10	Very sensitive
0.1-1	Moderately sensitive
0.01-0.1	Slightly sensitive
0-0.01	Insensitive

Table 10. Classification of the sensitivity of parameters according to their MAROV values

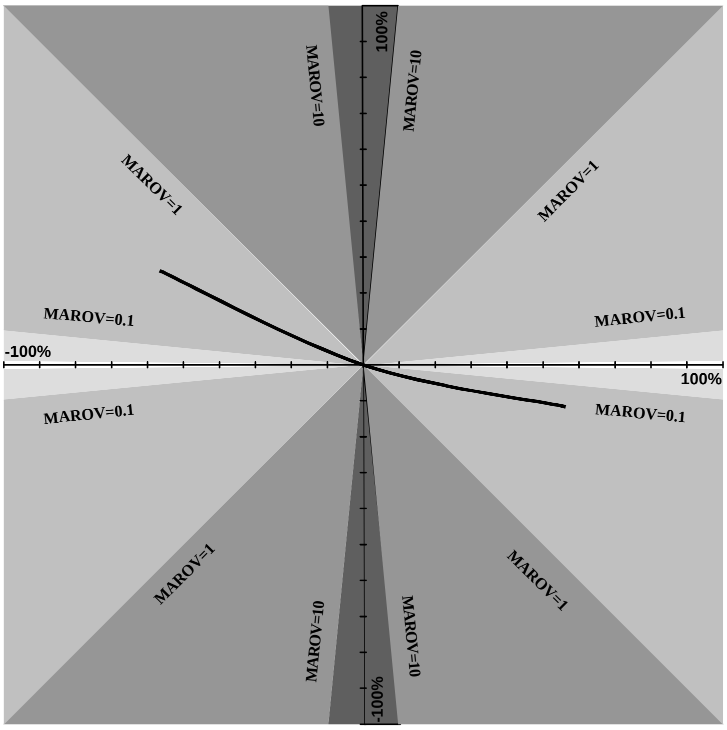

Figure 1. Graphical representation of MAROV values and the classes of sensitivity

The chart represents output variation (*y axis*) vs. input variation (*x axis*)

Classes of sensitivity are defined by lines which correspond to particular values of MAROV.

Extremely sensitive
Very sensitive
Moderately sensitive
Slightly sensitive
Insensitive

The line in the graphic represents the data for an input parameter which is “moderately sensitive”

The definition of the MAROV index might not be robust in some particular cases where the curves strongly deviate from linearity. This is exemplified in Figure 2a and 2b.

In Figure 2a, the MAROV index will be identical whichever the range of variation of the input parameter. In contrast, the MAROV index will be dependent on the range of variation for parameters which exhibit shapes similar to that presented in Figure 2b. In this particular case, the MAROV index will be the slope of the line joining the origin and point 4 (*i.e.* the largest slope for the four points). Non-linearity of the sensitivity curve might lead to an overestimation of sensitivity by the MAROV index under particular circumstances. Confidence in the ranking of parameters using the MAROV index can be gained by examining MAROV indices and sensitivity charts together.

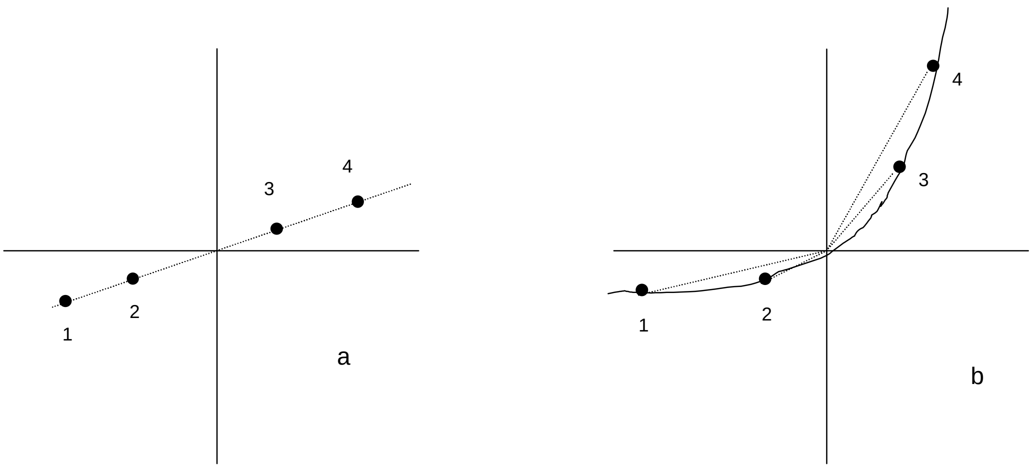

Figure 2. Charts explaining the derivation of the MAROV index from sensitivity curves
y-axis: variation in model output; x-axis: variation in model input
MAROV is defined as the steepest slope of the lines joining the origin and the different points

2.4. MONTE CARLO SENSITIVITY ANALYSIS

In contrast to one-at-a-time sensitivity analysis where parameters are varied one after the other, the Monte Carlo approach considers the variation of all input parameters at the same time. Values of input parameters are randomly selected in probability distribution functions describing the variability in input parameters.

2.4.1 Approach

A sensitivity analysis based on random sampling techniques includes the following steps:

- defining the model and its dependent and independent variables;
- assigning probability distribution functions to each input parameter;
- generating an input matrix through an appropriate random sampling method;
- running the model as many times as required to produce an output vector;
- assessing the influences and relative importance of each input/output relationship.

Although it is possible to specify correlations between different input parameters for the generation of probability distribution functions, this option was not used here since the information necessary to derive sound correlations between parameters was not readily available. Some relationships were nevertheless used, but outside the Monte Carlo sampling procedure. Values of parameters for the subsoil were linked to parameters in the topsoil.

Model results were related to input parameters by standardised regression analysis. This appears to be the most comprehensive technique for investigating model sensitivity and is relatively easy to perform with commercially available software (Hamby, 1994).

2.4.2 Attribution of probability distribution functions

Probability distribution functions (pdf's) were assigned according to the best estimates of the authors on the variation that would be expected for a particular parameter. For parameters that are measured in an unambiguous way, a symmetrical normal probability distribution was retained. Uncertain parameters which were attributed a variation factor of 2 in the sensitivity analysis were considered to be log-normally distributed. Finally, uniform distributions were attributed to a small number of parameters.

2.4.3 Statistical sampling

The traditional approach, referred to as "Monte Carlo", consists in sampling values purely randomly in the pdf's of input parameters. This usually implies a large number (> 10,000) of model runs and the approach is therefore extremely demanding for complex models with large running times (*e.g.* 10,000 simulations with a model which has a running time of 1 hour would keep a computer busy for more than one year).

The problem with the large number of runs that have to be carried out with the traditional Monte Carlo sampling has been addressed by McKay *et al.* (1979) who proposed a stratified random sampling scheme termed Latin Hypercube Sampling (LHS). In LHS, each probability distribution is divided into segments of equal area under the probability distribution function. Segments from each parameter distribution are sampled without replacement so that a segment is used in only one model run. For iteration, a parameter value is randomly selected from the randomly selected segment. Since all the segments of a parameter distribution contain equal area, the parameter can be sampled from a uniform distribution bounded by the limits of a segment. Also, the random sampling in most of the non-uniform distributions will often provide parameter values close to their means when using standard Monte Carlo sampling (Reed *et al.*, 1984). A more evenly distributed random sampling is obtained with LHS.

Rose (1983) showed that simple random sampling of 1000 runs and LHS of 200 runs provide similar results for a variety of statistical measures. Iman and Helton (1985) indicate that satisfactory results with LHS can be obtained by applying the following formula:

$N > 4/3 \times p$, where p is the number of parameters to be sampled.

The maximum number of parameters to be varied in the four leaching models was 43 (number of primary parameters for MACRO). Using this equation, the minimum number of runs to be carried out was thus 58 runs. It was decided to conduct 250 runs for all four models to improve confidence in the results.

2.4.4 Treatment of model results

Sensitivity of the models to changes in input parameters for Monte Carlo sampling was assessed using regression techniques. The principle of the technique is that the sensitivity of the model is proportional to the magnitude of regression coefficients (*i.e.* the larger the regression coefficient, the larger the sensitivity of the model to this particular parameter).

In a first stage, inputs and outputs were normalised because of unit discrepancies between parameters and the relative magnitude of parameters themselves. Regression coefficients obtained on this normalised data are often referred to as Standardised Regression Coefficients (SRC). The model of regression can be written as follows:

$$output\_s = \sum_i b_i \times input\_s_i + e$$

where *output_s* is the standardised output,
$input\_s_i$ is the standardised input,
b_i is the Standardised Regression Coefficient,
i is a coefficient describing the parameters,
e is the model error.

All terms of this equation are dimensionless.

One of the assumptions made when calculating regression statistics from the raw data is that the relationship between input and output is linear. This hypothesis is clearly not valid for complex models such as those describing leaching of pesticides. In order to reduce the impact of non-linearity, all data were replaced by their rank in the dataset (*i.e.* the largest value for a particular parameter was assigned the number 1, the second largest the number 2, etc.). This transformation is valid for our dataset because the relationship between input and output was shown to be monotonous in the one-at-a-time sensitivity analysis. The Rank Regression

Coefficients (RRC) or Standardised Rank Regression Coefficients (SRRC) were calculated by performing a regression analysis on rank-transformed standardised data rather than the raw standardised data. The model can be written:

$$ranked\_output\_s = \sum_i b_i \times ranked\_input\_s_i + e'$$

where ranked_*output_s* is the rank-transformed standardised output,

input_s$_i$ is the rank-transformed standardised input,

b_i is the Standardised Rank Regression Coefficient,

i is a coefficient describing the parameters,

e' is the model error.

3. RESULTS

***Preliminary note:* key for the designation of model runs**

In the following sections, scenarios are described using three letters (e.g. MTH, OLW, ZLH, ALW)

The first letter designates the model (M=MACRO, O=PELMO, Z=PRZM, A=PESTLA),

The second letter designates the pesticide (L or T),

The third letter designates the soil (W=Wick, H=Hodnet).

3.1 MACRO 4.1

3.1.1 Results for the four scenarios (the four "base-cases")

The four base-cases resulted from modelling the fate of the two pesticides with contrasting properties in the two contrasting soil types. Percolation and pesticide losses for the four scenarios are presented in Table 11 (annual data) and Table 12 (accumulated values).

Predicted percolation for the two soils was very similar (annual difference of 12 mm in the prediction of percolation volumes). Total pesticide losses were predicted to range from 33.8 to 39.8 g/ha (Pesticide L) and from 7.5 to 87.3 g/ha (Pesticide T). Predicted losses for both pesticides were larger in the clay loam (Hodnet) than in the sandy loam (Wick), especially for pesticide T (87.3 g/ha compared to 7.5 g/ha, respectively). This reflects greater leaching by preferential flow in the more highly structured Hodnet soil. In the Wick soil, losses of pesticide L were predicted to be larger than those of pesticide T. In the Hodnet soil, the reverse was predicted. This highlights the complex interactions between the molecule and the soil environment and, again, the influence of considering preferential flow processes in leaching modelling.

	Percolation (mm)				Pesticide losses at 1-m depth (g/ha)			
	MLW	MTW	MLH	MTH	MLW	MTW	MLH	MTH
1985	242	242	230	230	0.02	<0.01	23.87	51.06
1986	283	283	271	271	29.80	1.45	15.83	33.61
1987	283	283	271	271	3.99	4.10	0.11	2.47
1988	286	286	273	273	0.01	1.60	<0.01	0.15
1989	-	283	-	-	-	0.32	-	-
1990	-	283	-	-	-	0.05	-	-

Table 11. Annual percolation and cumulated pesticide losses predicted by MACRO for the four scenarios

	MLW	MTW	MLH	MTH
Number of years to achieve full breakthrough	4	6	4	4
Total percolation (mm)	1094	1660	1045	1045
Total pesticide losses at 1-m depth (g/ha)	33.82	7.52	39.80	87.29
Total pesticide losses at 1-m depth (% applied)	1.69	0.38	1.99	4.36

Table 12. Accumulated percolation and pesticide losses predicted by MACRO for the four scenarios

Figure 3 presents daily pesticide losses predicted by the MACRO model for each scenario. Leaching breakthrough was dependent on the soil considered. In the Wick soil (scenarios MLW and MTW), losses by percolation occurred over relatively long time periods (*e.g.* over 7.5 and 5 months for the two events of the scenario MLW). Leaching happened over 2 years for pesticide L and 4 years for pesticide T. In contrast, pesticide losses from the more structured Hodnet soil were short-lived and dominated by transient peaks in a single year with much larger daily losses. Maximum daily losses were 10 and 209 times larger in the clay loam than in the sandy loam for pesticide L and T, respectively. Transient losses are typical of soils with preferential flow.

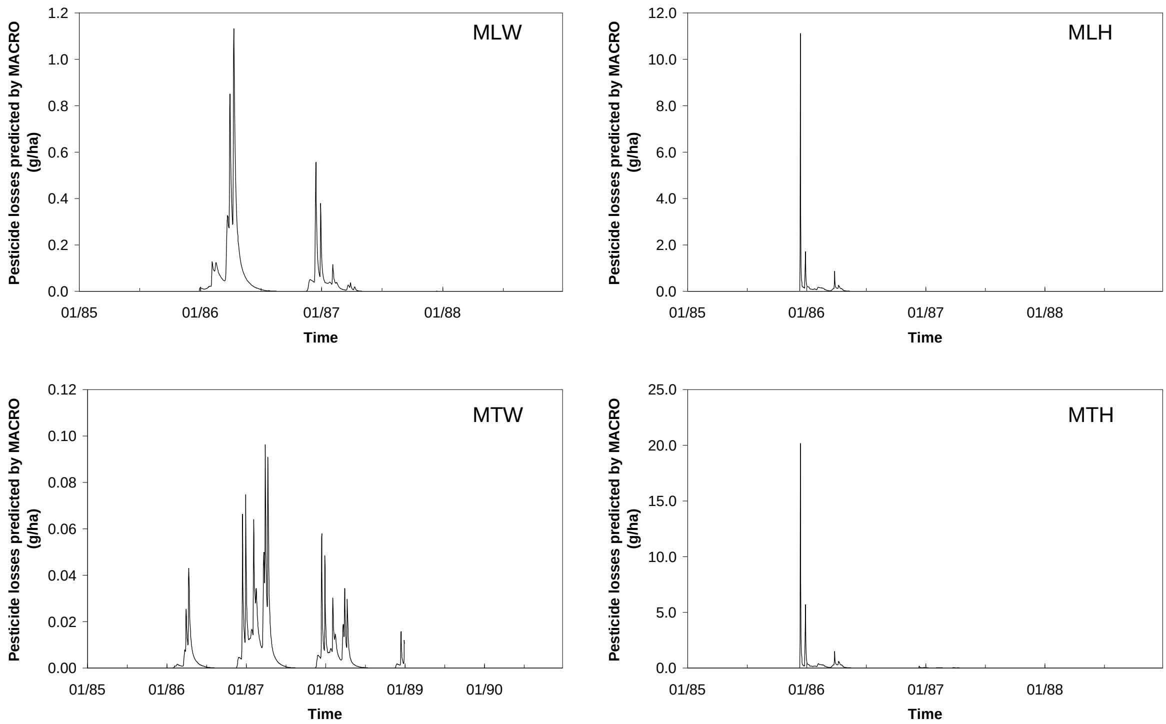

Figure 3. Daily pesticide losses predicted by MACRO for the four scenarios (g/ha)

3.1.2 Results for the one-at-a-time sensitivity analysis

A total of 1426 runs were carried out to assess the one-at-a-time sensitivity of MACRO to the 43 primary parameters for the four scenarios.

The results of the influence of input parameters on the prediction of percolation and pesticide losses are presented graphically in Appendices 8 to 15. Examples of charts for the MLW scenario are presented in Figures 4 and 5. These charts present the variation in the model output (either percolation or pesticide losses) vs. the variation in the input. Values on the two axes are percentages, which mean that direct comparison of the influence of the different parameters can be made. The closer the curve to the Y-axis, the more influence a particular parameter has. Parameters which have a curve located in the top right or bottom left quadrants have a "positive" influence on model results (*i.e.* an increase in the value of the input will result in an increase in the value of the output). In contrast, an increase in the values of input parameters which have a curve in the top left or bottom right quadrants will result in a decrease in the model output ("negative" influence).

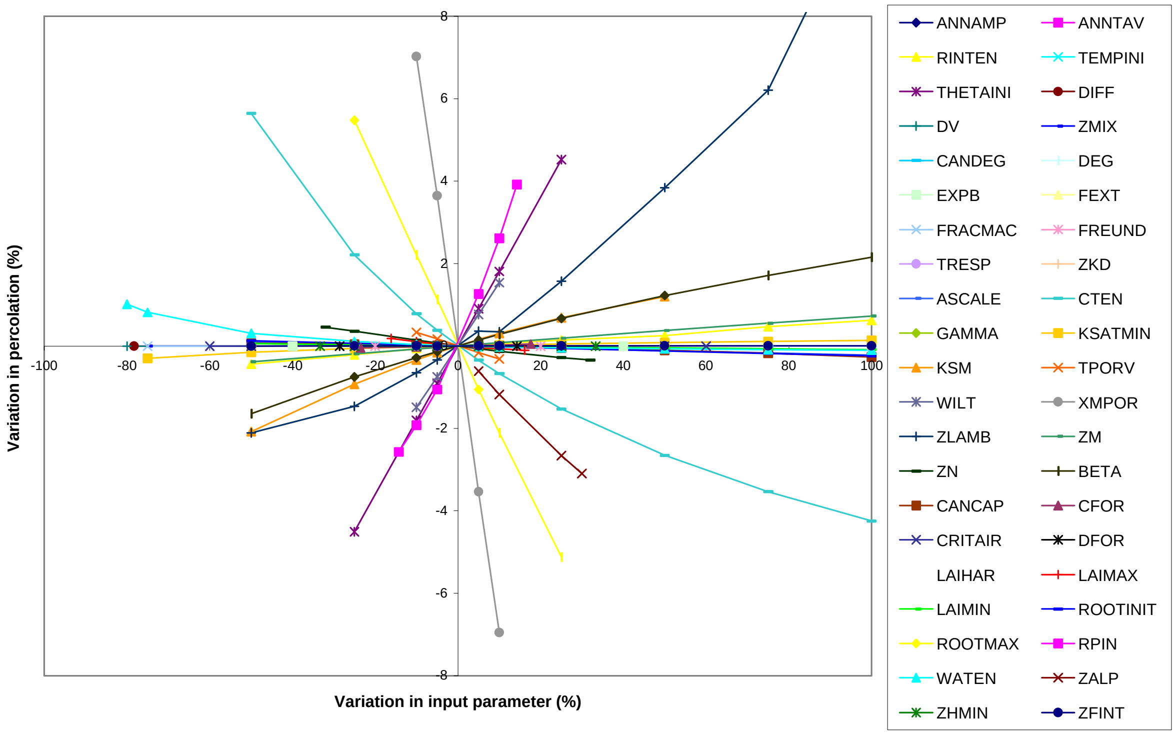

Figure 4. Influence of the variation of input parameters on percolation predicted by MACRO for the MLW (Pesticide L on Wick) scenario

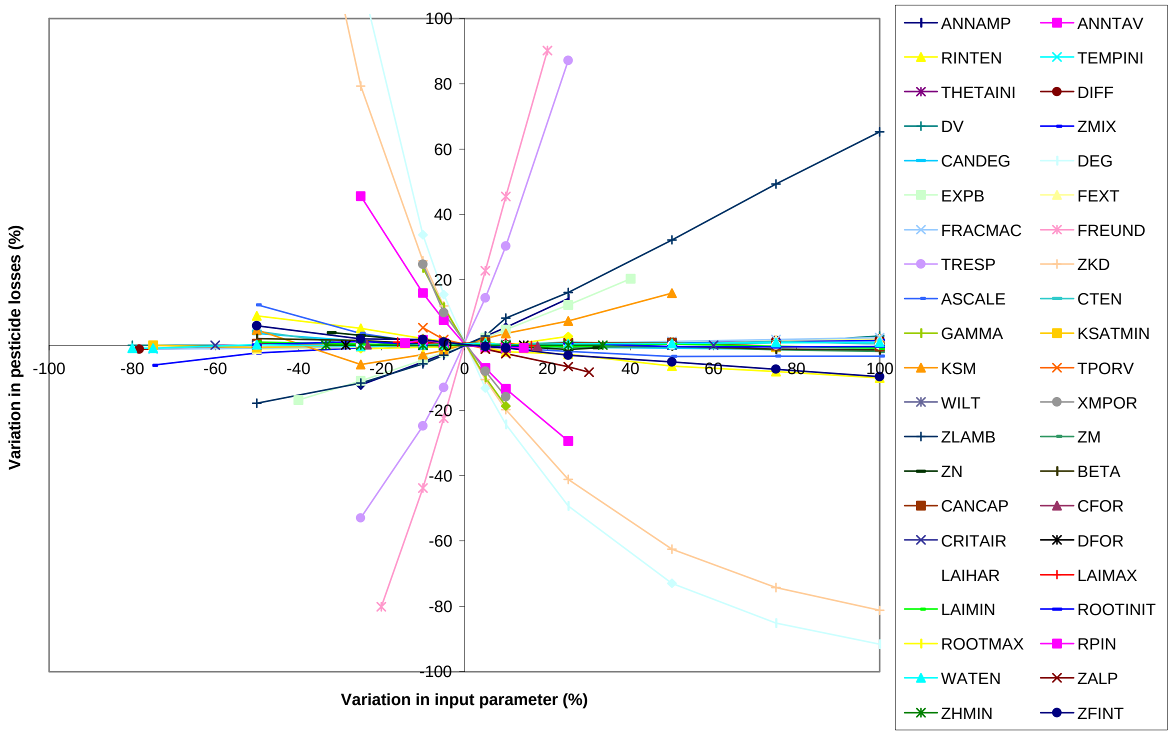

Figure 5. Influence of the variation of input parameters on pesticide losses predicted by MACRO for the MLW (Pesticide L on Wick) scenario

For comparison and classification purposes, the sensitivity of the model to individual parameters was also quantified using the MAROV index. MAROV values for individual scenarios are reported in Appendices 16 to 23. Results aggregated for all scenarios are reported in Table 13 for percolation and in Table 14 for pesticide losses. In these two tables, parameters are classified according to the mean MAROV for the four scenarios for each parameter. Parameters which have the most influence on prediction of percolation and pesticide losses (larger MAROV values) can be found at the top of the tables.

		Wick				Hodnet				
		Pesticide L		Pesticide T		Pesticide L		Pesticide T		Influence
XMPOR	Boundary soil water content	0.728	-	0.728	-	0.856	-	0.856	-	-
RPIN	Root distribution	0.274	+	0.274	+	0.371	+	0.371	+	+
THETAINI	Initial soil moisture	0.181	+	0.181	+	0.320	+	0.320	+	+
ROOTMAX	Max root depth	0.226	-	0.226	-	0.280	-	0.280	-	-
WILT	Wilting point	0.153	+	0.153	+	0.300	+	0.300	+	+
TPORV	Saturated water content	0.034	-	0.034	-	0.236	-	0.236	-	-
ZALP	Correction factor for wet canopy evaporation	0.122	-	0.122	-	0.133	-	0.133	-	-
CTEN	Boundary soil water tension	0.113	-	0.113	-	0.095	-	0.095	-	-
ZLAMB	Pore size distribution index	0.114	+	0.114	+	0.054	+/-	0.054	+/-	+/-
BETA	Root adaptability factor	0.033	+	0.033	+	0.054	+	0.054	+	+
ZN	Pore size distribution factor macrop.	0.014	-	0.014	-	0.049	-	0.049	-	-
GAMMA	Bulk density	0.012	-	0.012	-	0.021	-	0.021	-	+/-
KSM	Boundary hydraulic conductivity	0.042	+	0.042	+	0.005	+/-	0.005	+/-	+/-
LAIMAX	Max Leaf Area Index	0.011	-	0.011	-	0.018	-	0.018	-	-
KSATMIN	Saturated hydraulic conductivity	0.004	+	0.004	+	0.015	+	0.015	+	+
WATEN	Critical water tension for root water uptake	0.013	-	0.013	-	0.005	-	0.005	-	-
RINTEN	Rainfall intensity	0.009	+	0.009	+	0.007	+	0.007	+	+
ZM	Tortuosity factor micropores	0.008	+	0.008	+	0.005	+	0.005	+	+
CFORM	Form factor	0.002	+	0.002	+	0.004	+	0.004	+	+
ROOTINIT	Root Depth at zdatemin	0.003	-	0.003	-	0.003	-	0.003	-	-
CANCAP	Canopy Interception Capacity	0.003	-	0.003	-	0.002	-	0.002	-	-
ASCALE	Effective diffusion pathlength	0.002	-	0.002	-	0.002	-	0.002	-	-
LAIMIN	Leaf Area Index at zdatemin	0.001	-	0.001	-	0.002	-	0.002	-	-
CRITAIR	Critical soil air content for root water uptake	0		0		0.001	+	0.001	+	+
ZFINT	Fraction of irrigation intercepted by canopy	0		0		0		0		
ANNAMP	Temp annual amplitude	0		0		0		0		
ANNTAV	Average annual temp	0		0		0		0		
TEMPINI	Initial soil temp	0		0		0		0		
DIFF	Diffusion coefficient in water	0		0		0		0		
DV	Dispersivity	0		0		0		0		
ZMIX	Mixing depth	0		0		0		0		
CANDEG	Canopy degradation rate	0		0		0		0		
DEG	Degradation rates	0		0		0		0		
EXPB	Exponent moisture relation	0		0		0		0		
FEXT	Canopy wash-off coefficient	0		0		0		0		
FRACMAC	Fraction sorption sites macropores	0		0		0		0		
FREUND	Freundlich exponent	0		0		0		0		
TRESP	Exponent Temp response	0		0		0		0		
ZKD	Sorption coefficient	0		0		0		0		
DFORM	Form factor	0		0		0		0		
LAIHAR	Leaf Area Index at harvest	0		0		0		0		
ZHMIN	Crop height at zdatemin	0		0		0		0		

Table 13. Classification of MACRO parameters according to their influence on percolation (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase in percolation and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive

Very sensitive

Moderately sensitive

Slightly sensitive

Insensitive

		Wick				Hodnet				
		Pesticide L		Pesticide T		Pesticide L		Pesticide T		Influence
FREUND	Freundlich exponent	4.552	+	22.21	+	1.348	+	2.070	+	+
DEG	Degradation rates	8.157	-	11.94	-	3.097	-	1.218	-	-
ZKD	Sorption coefficient	4.496	-	12.13	-	0.242	-	0.633	-	-
TPORV	Saturated water content	0.524	-	5.895	-	2.696	-	6.675	-	-
KSM	Boundary hydraulic conductivity	0.389	+/-	7.000	-	1.247	-	1.619	-	+/-
TRESP	Exponent Temp response	3.488	+	3.369	+	1.765	+	0.722	+	+
ZN	Pore size distribution factor macrop.	0.131	-	5.615	-	0.818	-	2.739	-	-
XMPOR	Boundary soil water content	2.469	-	0.948	+	0.938	+	2.273	+	+/-
GAMMA	Bulk density	2.363	-	3.680	-	0.067	-	0.448	-	-
ANNTAV	Average annual temp	1.823	-	2.231	-	0.597	-	0.406	-	-
ASCALE	Effective diffusion pathlength	0.247	-	0.873	+	0.692	+	1.504	+	+/-
ZLAMB	Pore size distribution index	0.829	+	1.450	-	0.456	-	0.341	-	+/-
KSATMIN	Saturated hydraulic conductivity	0.147	+/-	0.631	+	0.267	+	0.549	+	+/-
EXPB	Exponent moisture relation	0.507	+	0.855	+	0.056	+	0.034	+/-	+/-
RINTEN	Rainfall intensity	0.232	-	0.950	+	0.091	+/-	0.124	+	+/-
CTEN	Boundary soil water tension	0.085	+/-	0.868	-	0.069	+/-	0.272	-	+/-
ANNAMP	Temp annual amplitude	0.568	+	0.362	+	0.222	+	0.128	+	+
DIFF	Diffusion coefficient in water	0.019	+	0.067	-	0.302	-	0.826	-	+/-
ROOTMAX	Max root depth	0.188	+/-	0.336	+	0.366	-	0.290	-	+/-
RPIN	Root distribution	0.157	-	0.414	-	0.322	+	0.211	+	+/-
WILT	Wilting point	0.125	-	0.248	-	0.363	+	0.255	+	+/-
ZALP	Correction factor for wet canopy evaporation	0.276	-	0.293	-	0.101	-	0.146	-	-
FRACMAC	Fraction sorption sites macropores	0.023	+	0.481	-	0.043	+	0.245	-	+/-
ZFINT	Fraction of irrigation intercepted by canopy	0.193	-	0.165	-	0.104	-	0.067	-	-
ZMIX	Mixing depth	0.082	+	0.218	+	0.026	+/-	0.137	+	+/-
CANCAP	Canopy Interception Capacity	0.183	+/-	0.126	+/-	0.126	+/-	0.029	+/-	+/-
WATEN	Critical water tension for root water uptake	0.132	+/-	0.080	+/-	0.136	+/-	0.065	+/-	+/-
BETA	Root adaptability factor	0.132	+/-	0.119	-	0.112	+	0.038	+/-	+/-
THETAINI	Initial soil moisture	0.085	+/-	0.141	+/-	0.152	+/-	0.012	+/-	+/-
ZM	Tortuosity factor micropores	0.113	+/-	0.112	+/-	0.065	+/-	0.023	+/-	+/-
CANDEG	Canopy deg rate	0.070	-	0.062	-	0.122	-	0.052	-	-
LAIMIN	Leaf Area Index at zdatemin	0.079	+/-	0.111	+/-	0.051	+/-	0.022	-	+/-
ROOTINIT	Root Depth at zdatemin	0.056	+/-	0.087	+/-	0.064	+/-	0.051	+/-	+/-
DV	Dispersivity	0.134	+	0.050	-	0.007	+/-	0.053	-	+/-
LAIMAX	Max Leaf Area Index	0.092	+/-	0.053	+/-	0.037	+/-	0.041	+/-	+/-
CFORM	Form factor	0.050	+/-	0.064	+/-	0.054	+/-	0.035	+/-	+/-
FEXT	Canopy wash-off coefficient	0.026	+	0.054	+	0.029	+	0.046	+	+
CRITAIR	Critical soil air for root water uptake	0		0		0.092	+/-	0.033	+/-	+/-
TEMPINI	Initial soil temp	0		0		0		0		
DFORM	Form factor	0		0		0		0		
LAIHAR	Leaf Area Index at harvest	0		0		0		0		
ZHMIN	Crop height at zdatemin	0		0		0		0		

Table 14. Classification of MACRO parameters according to their influence on <u>pesticide losses</u> (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase in pesticide losses and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive
Very sensitive
Moderately sensitive
Slightly sensitive
Insensitive

The sensitivity of percolation to input parameters in MACRO is presented in Table 13. Maximum MAROV values for percolation were all below 1 (maximum 0.86), which means that a particular variation in an input would result in a smaller variation in the predicted percolation. No notable difference was found in the ranking of parameters between the four scenarios.

The parameter which had the most influence on percolation volumes was XMPOR, the boundary soil water content. This parameter is one the three parameters (CTEN, XMPOR and KSM) which define the boundary between micropores and macropores in MACRO. In this study, these three parameters were varied independently, but as the three parameters are numerically linked, a refinement of the study could include a variation of the three parameters at the same time.

Parameters related to the description of soil water content (THETAINI, WILT, XMPOR and TPORV) were found to have a small influence on percolation results (maximum MAROV value 0.32). The use of water retention data specific to the soil used is desirable to achieve a good description of water flow processes in soil. Also, the influence of the initial soil moisture content (THETAINI) emphasises that a pre-run of a few months or years should be carried out to allow equilibration of the model with respect to water content in the soil profile.

Two crop parameters were listed in the five most influential parameters for percolation: RPIN, the root distribution percentage and ROOTMAX, the maximum rooting depth, which are two parameters related to the description of the root system of the crop. RPIN represents the percentage of root length in the top 25% of the root depth. Variation of other crop parameters were found to have little effect on percolation results.

No meteorological data were included in the sensitivity analysis because these parameters were considered as certain within the scope of this study. This is not the case in practice since there is evidence of large measurements errors in meteorological datasets. Potential evapotranspiration (PET) is uncertain because different values are produced by different methods or different individuals. Given the small magnitude of MAROV values found for percolation, the balance of PET minus rainfall is expected to be the most influential variable for percolation predictions.

The influence of a change in model input on model output was occasionally dependent on the values which were selected within a scenario (+/- signs in Table 13). For instance, an increase by 5% in the bulk density GAMMA resulted in a decrease in percolation volumes whereas an increase by 10% resulted in an increase in percolation.

The sensitivity of **pesticide losses** to input parameters in MACRO is presented in Table 14 and the 15 most influential parameters by scenario are reported in Table 15.

	MLW		MTW		MLH		MTH	
1	DEG	8.157	FREUND	22.211	DEG	3.097	TPORV	6.675
2	FREUND	4.552	ZKD	12.129	TPORV	2.696	ZN	2.739
3	ZKD	4.496	DEG	11.942	TRESP	1.765	XMPOR	2.273
4	TRESP	3.488	KSM	7.000	FREUND	1.348	FREUND	2.070
5	XMPOR	2.469	TPORV	5.895	KSM	1.247	KSM	1.619
6	GAMMA	2.363	ZN	5.615	XMPOR	0.938	ASCALE	1.504
7	ANNTAV	1.823	GAMMA	3.680	ZN	0.818	DEG	1.218
8	ZLAMB	0.829	TRESP	3.369	ASCALE	0.692	DIFF	0.826
9	ANNAMP	0.568	ANNTAV	2.231	ANNTAV	0.597	TRESP	0.722
10	TPORV	0.524	ZLAMB	1.450	ZLAMB	0.456	ZKD	0.633
11	EXPB	0.507	RINTEN	0.950	ROOTMAX	0.366	KSATMIN	0.549
12	KSM	0.389	XMPOR	0.948	WILT	0.363	GAMMA	0.448
13	ZALP	0.276	ASCALE	0.873	RPIN	0.322	ANNTAV	0.406
14	ASCALE	0.247	CTEN	0.868	DIFF	0.302	ZLAMB	0.341
15	RINTEN	0.232	EXPB	0.855	KSATMIN	0.267	ROOTMAX	0.290

Table 15. The 15 most influential parameters on the prediction of pesticide losses by MACRO for the four scenarios (classification by MAROV values).

Maximum MAROV values for pesticide losses ranged from 3.1 (Pesticide L on Hodnet soil) to 22.2 (Pesticide T on Wick soil). The ranking of the most influential parameters was found to be influenced by both the soil type and the compound, and large differences were found. For example, ZN, the pore size distribution index was found to be the second most influential parameter in the MTH scenario whereas it was ranked 24th in the MLW scenario.

In the Wick soil which is coarser textured and more weakly structured than the Hodnet soil, MACRO was most sensitive to three parameters related to the degradation (degradation rates) or sorption (Freundlich coefficient and exponent) of pesticides. The importance of these parameters was particularly great for pesticide T where the parameters had MAROV values above 10 (a value of 10 means that an increase of 10% in the input parameter will double the value of the output). Following these three dominant parameters (and TRESP, the parameter which describes the influence of temperature on degradation kinetics, for the MLW scenario), the next most influential inputs were related to the description of the soil hydrology and the soil (KSM, XMPOR, ZN, GAMMA).

Sensitivities of pesticide losses predicted by MACRO in the Hodnet soil were less than those reported for the Wick soil for both pesticides. In the Hodnet soil, the MACRO model was much more influenced by hydrological parameters than was shown for the Wick soil, even if parameters related to degradation and sorption still dominated in the scenario with pesticide L. TPORV (the water content at saturation) was the most and second most influential parameter for the MTH and MLH scenarios, respectively. In the scenario with pesticide T, five out of the six top parameters were hydrological parameters. The second most influential parameter (ZN, tortuosity factor for the macropores) of the MTH scenario is particularly uncertain because it cannot be determined experimentally and very little guidance is available; this might lead to large discrepancies in model results from different users. The presence of the diffusion coefficient in water (DIFF) in the top 10 parameters is also specific to the MTH scenario. Although the sorption coefficient was found to greatly influence results for pesticide losses in the Wick soil (ranked 2 and 3), its influence was much less pronounced in the Hodnet soil (ranked 10 and 16).

The impact of a change in some inputs resulted in either a decrease or an increase in pesticide losses depending on the scenario considered (*e.g.* ASCALE, ZLAMB, Table 14) or the values that were taken by a parameter within a scenario (*e.g.* CANCAP, WATEN, or most crop parameters). The change of influence was sometimes attributed to a specific compound (*e.g.* FRACMAC) or to a specific soil (*e.g.* RPIN). The fact that a change in the input has different impacts on model results is due to the combination of different processes combined in the model.

3.1.2 Results for the Monte Carlo sensitivity analysis

Input parameters obtained from sampling in the different probability distributions are presented in Appendices 34 to 37. A total of 250 runs were carried out. Basic statistics on the percolation and pesticide losses predicted by MACRO are presented in Table 16. More detailed statistics can be found in Appendices 38 to 47.

	Percolation (mm)				Pesticide losses (g/ha)			
	MLW	MTW	MLH	MTH	MLW	MTW	MLH	MTH
Minimum	914	1384	776	872	0.0	0.0	1.5	0.1
Mean	1084	1643	1040	1039	58.5	24.1	44.6	93.8
Median	1084	1647	1042	1045	38.8	10.9	37.5	79.4
Maximum	1291	1970	1209	1222	336.0	249.2	128.0	275.7
CV (%)	6.1	5.7	7.2	6.9	100	149	61	69

Table 16. Basic statistics on MACRO predictions for the four scenarios using input parameters generated by Monte Carlo sampling

Regression techniques were used for non-transformed standardised data and transformed (ranked) standardised data (see section 2.4.4). Coefficients of determination related to pesticide losses for the transformed data (r^2 0.92-0.95) were significantly larger than those for non-transformed data (r^2 0.68-0.90) because of the non-linearity inherent in the computation of pesticide losses by MACRO. It was therefore decided to restrict the analysis of the sensitivity of the model to Standardised Rank Regression Coefficients (SRRC). Results of the regressions are presented in Table 17 for percolation and Table 18 for pesticide losses. The larger the absolute values of the regression coefficients (SRRC) the more influence the parameter has. An increase in a parameter with a positive coefficient will result in an increase in the model output and vice versa.

	MLW		MTW		MLH		MTH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
XMPOR	-0.579	1	-0.494	1	-0.473	2	-0.500	2
ROOTMAX	-0.415	2	-0.442	2	-0.409	3	-0.413	3
THETAINI	0.307	5	0.228	5	0.481	1	0.506	1
CTEN	-0.373	3	-0.372	3	-0.240	5	-0.253	5
RPIN	0.242	6	0.224	6	0.265	4	0.260	4
WILT	0.118	9	0.117	9	0.159	6	0.204	6
BETA	0.091	10	0.149	7	0.152	7	0.173	7
ZLAMB	0.309	4	0.330	4	-0.075	12	-0.063	12
ZALP	-0.167	7	-0.140	8	-0.136	8	-0.135	9
CANCAP	-0.050	11	-0.047	13	-0.079	11	-0.028	17
ZM	0.028	21	0.043	14	0.060	13	0.040	15
TPORV	0.008	34	-0.039	16	-0.130	9	-0.146	8
FREUND	0.037	15	0.062	11	-0.012	33	0.016	25
KSM	0.132	8	0.086	10	0.016	28	-0.002	41
WATEN	0.016	26	-0.025	20	-0.012	32	-0.074	11
ANNAMP	-0.043	12	0.020	26	0.020	26	-0.015	27
CANDEG	0.036	17	-0.017	32	-0.028	23	-0.024	19
ZN	0.009	33	-0.005	40	-0.084	10	-0.089	10
LAIMIN	0.016	27	-0.013	35	-0.037	19	-0.050	13
RINTEN	0.000	43	0.055	12	0.032	20	0.023	20
DV	-0.035	18	-0.024	21	0.038	17	0.002	42
LAIMAX	-0.016	28	0.020	28	-0.054	14	-0.014	29
CFORM	0.028	22	0.033	17	0.025	24	-0.009	37
DFORM	-0.013	30	0.024	22	-0.037	18	-0.011	30
FEXT	-0.038	13	0.016	33	-0.030	22	0.010	33
ASCALE	-0.014	29	0.040	15	-0.005	39	0.022	21
ZFINT	-0.037	16	0.018	30	-0.045	15	-0.001	43
DIFF	0.000	42	-0.026	19	0.013	30	-0.044	14
CRITAIR	0.002	40	-0.019	29	0.043	16	0.018	23
ROOTINIT	-0.033	19	-0.021	24	-0.004	40	0.015	28
EXPB	-0.018	24	0.021	25	-0.009	37	0.015	26
FSTAR	-0.002	39	-0.029	18	-0.031	21	0.009	36
KSATMIN	0.012	31	0.011	36	0.015	29	0.028	18
FRACMAC	-0.025	23	0.001	43	0.016	27	0.016	24
ZKD	0.037	14	-0.020	27	-0.003	41	-0.009	35
ZMIX	0.004	35	0.017	31	-0.003	42	-0.032	16
ZHMIN	0.012	32	-0.023	23	0.005	38	-0.010	34
DEG	0.002	38	0.001	42	0.012	31	0.021	22
TEMPINI	0.001	41	-0.010	37	0.024	25	0.010	31
GAMMA	0.017	25	-0.005	41	-0.011	35	0.006	38
LAIHAR	-0.032	20	-0.009	38	0.002	43	-0.004	39
TRESP	0.004	36	0.006	39	-0.010	36	-0.010	32
ANNTAV	0.003	37	-0.015	34	-0.011	34	0.003	40

Table 17. Classification of MACRO input parameters according to their influence on results for percolation (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

	MLW		MTW		MLH		MTH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
DEG	-0.648	1	-0.479	3	-0.730	1	-0.286	4
FREUND	0.292	3	0.523	1	0.170	6	0.261	5
TRESP	0.287	4	0.182	6	0.331	2	0.110	10
ZKD	-0.483	2	-0.484	2	-0.092	11	-0.214	7
KSM	0.030	15	-0.210	4	-0.268	3	-0.345	2
ZLAMB	0.104	6	-0.097	8	-0.162	8	-0.131	9
ZN	-0.022	21	-0.210	5	-0.208	4	-0.294	3
ANNTAV	-0.144	5	-0.110	7	-0.114	9	-0.032	22
ASCALE	-0.013	28	0.082	9	0.179	5	0.463	1
KSATMIN	-0.019	22	0.075	11	0.059	12	0.081	14
TPORV	-0.008	34	-0.057	16	-0.167	7	-0.205	8
XMPOR	-0.048	10	0.020	28	0.051	13	0.081	15
RINTEN	-0.024	18	0.071	12	-0.006	35	0.089	12
FRACMAC	0.014	27	-0.066	14	-0.018	26	-0.099	11
EXPB	0.055	8	0.082	10	0.005	38	0.028	24
GAMMA	-0.036	12	-0.068	13	-0.006	36	-0.035	21
CTEN	-0.004	39	-0.051	17	-0.050	15	-0.082	13
ZFINT	-0.047	11	-0.026	27	0.014	29	-0.053	17
ZMIX	-0.034	14	-0.006	36	-0.020	24	0.060	16
DIFF	0.003	41	-0.007	34	-0.100	10	-0.235	6
FSTAR	-0.060	7	0.033	22	0.013	30	0.003	41
CANCAP	0.026	17	0.001	42	0.021	23	0.048	18
DV	-0.013	30	0.017	30	-0.020	25	-0.046	19
ANNAMP	0.022	20	-0.005	38	0.050	14	0.011	34
WILT	-0.052	9	-0.006	35	-0.023	21	0.001	43
ZM	-0.035	13	-0.003	39	-0.014	28	-0.020	28
ROOTINIT	0.006	35	0.063	15	0.008	34	0.021	27
CANDEG	0.005	37	0.036	21	-0.034	17	-0.004	38
DFORM	0.010	33	0.007	33	0.030	18	0.016	31
LAIMAX	0.006	36	-0.039	20	-0.004	39	-0.038	20
ZALP	-0.013	29	0.050	18	-0.010	32	0.010	36
CFORM	-0.016	24	-0.018	29	0.009	33	0.017	30
LAIHAR	-0.016	25	-0.040	19	0.000	43	-0.017	29
RPIN	0.011	32	-0.031	24	0.025	19	0.003	42
ZHMIN	-0.023	19	-0.012	31	0.000	42	-0.024	26
THETAINI	-0.027	16	-0.030	25	-0.001	41	0.009	37
ROOTMAX	-0.003	40	0.007	32	-0.021	22	0.025	25
WATEN	-0.016	23	0.005	37	-0.023	20	-0.004	39
LAIMIN	0.004	38	0.001	43	-0.042	16	-0.030	23
FEXT	0.001	43	0.031	23	0.014	27	0.012	33
TEMPINI	-0.011	31	-0.026	26	-0.002	40	0.011	35
BETA	-0.015	26	-0.002	41	0.006	37	-0.003	40
CRITAIR	0.002	42	-0.003	40	-0.011	31	0.013	32

Table 18. Classification of MACRO input parameters according to their influence on results for pesticide losses (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

Again, as for the one-at-a-time sensitivity analysis, the impact of changes in model input on model output (*i.e.* the sign of SRRC in Tables 17 and 18) sometimes depended on the scenario considered. Although these differences are probably mostly genuine, they might also be partly attributed to the approximation of the relationship between model input and output by a regression analysis. In contrast to the one-at-a-time sensitivity analysis where MACRO was most sensitive to XMPOR in all four scenarios, the most influential parameters as determined by Monte Carlo sensitivity analysis are XMPOR (scenarios with the Wick) and THETAINI (scenarios with the Hodnet). THETAINI is the soil moisture content at the beginning of the modelling period and this influences the water regime in the first few days to few months of the simulation. For this reason, most modelling exercises are carried out with a few months of simulation before the application of a product to allow for the equilibration of soil moisture. Using this particular approach, this parameter does not have any influence on flow regime or pesticide losses once soil moisture is equilibrated across the profile.

Table 19 presents a list of the parameters that most influence pesticide losses predicted by MACRO. Again, as for the one-at-a-time sensitivity analysis, the model was most sensitive to degradation and sorption parameters for the Wick scenarios. For the scenario involving the pesticide L in the Hodnet soil, predictions of pesticide losses were mostly influenced by degradation parameters. In contrast, pesticide losses were mainly governed by soil hydrological parameters for the scenario involving pesticide T and the Hodnet soil.

	MLW		MTW		MLH		MTH	
1	DEG	-0.648	FREUND	0.523	DEG	-0.730	ASCALE	0.463
2	ZKD	-0.483	ZKD	-0.484	TRESP	0.331	KSM	-0.345
3	FREUND	0.292	DEG	-0.479	KSM	-0.268	ZN	-0.294
4	TRESP	0.287	KSM	-0.210	ZN	-0.208	DEG	-0.286
5	ANNTAV	-0.144	ZN	-0.210	ASCALE	0.179	FREUND	0.261
6	ZLAMB	0.104	TRESP	0.182	FREUND	0.170	DIFF	-0.235
7	FSTAR*	-0.060	ANNTAV	-0.110	TPORV	-0.167	ZKD	-0.214
8	EXPB	0.055	ZLAMB	-0.097	ZLAMB	-0.162	TPORV	-0.205
9	WILT	-0.052	ASCALE	0.082	ANNTAV	-0.114	ZLAMB	-0.131
10	XMPOR	-0.048	EXPB	0.082	DIFF	-0.100	TRESP	0.110
11	ZFINT	-0.047	KSATMIN	0.075	ZKD	-0.092	FRACMAC	-0.099
12	GAMMA	-0.036	RINTEN	0.071	KSATMIN	0.059	RINTEN	0.089
13	ZM	-0.035	GAMMA	-0.068	XMPOR	0.051	CTEN	-0.082
14	ZMIX	-0.034	FRACMAC	-0.066	ANNAMP	0.050	KSATMIN	0.081
15	KSM	0.030	ROOTINIT	0.063	CTEN	-0.050	XMPOR	0.081

* FSTAR was not included in the one-at-a-time sensitivity analysis

Table 19. The 15 most influential parameters on the prediction of pesticide losses by MACRO for the four scenarios (Monte Carlo sampling).

Parameters are classified according to Standardised Rank Regression Coefficients (SRRC).

There were some significant differences in the lists of parameters generated by one-at-a-time and Monte Carlo sensitivity analysis. This is not surprising since the detailed results of a sensitivity analysis depend on the method which is used. Actual coefficients or a strict adherence to sensitivity ranking are not as important as the determination of the top few parameters to which the model is most sensitive (Hamby, 1994).

Sensitivity analysis techniques based on Monte Carlo sampling and regression analysis are often recommended for investigating the sensitivity of models with a large number of parameters because they are not very computer-intensive. It is nevertheless felt that the techniques carry a number of shortcomings. For the current study, the main problem arose from the use of regression techniques which cannot describe the relationship between model output and inputs in, non linear, pesticide fate models ($r^2<1$). Regression coefficients were therefore an inadequate description of this relationship and a comparison of these coefficients is questionable. A clear example is that the sign of some regression coefficients for parameters which have little influence on model results change according to the different scenarios (*e.g.* ZMIX or FEXT for the prediction of percolation, Appendix 56). Furthermore, the regression generated a coefficient for all input parameters, even those which were shown to have no influence on model output in the one-at-a-time sensitivity analysis (*e.g.* percolation results should not be affected by parameters related to sorption or degradation). The attribution of non-zero regression coefficients to parameters which do not have an influence on model results obviously affected other parameters and the whole approach could therefore be flawed. A solution to this particular problem would be to only include those parameters that have been shown to influence model results, but these techniques would lose some of their advantages if a one-at-a-time sensitivity analysis had to be performed beforehand.

3.2 PELMO 3.00

3.2.1 Results for the four scenarios (the four "base-cases")

Tables 20 and 21 present annual and cumulative percolation and losses of pesticides simulated by PELMO for the four scenarios. Predicted percolation was similar for the two scenarios (annual difference 18 mm). Total pesticide losses were predicted to be 25.7 g/ha for pesticide L in the Wick soil, but much smaller for the other pesticide-soil combinations. Virtually no leaching was predicted for the fourth scenario (Pesticide T on Hodnet, total losses of 5.5×10^{-6} g/ha). Losses were predicted to be larger for pesticide L compared to pesticide T. Also, for a given molecule, predicted losses were larger in the sandy loam (Wick) than in the more structured clay loam (Hodnet). PELMO does not include a description of preferential flow.

	Percolation (mm)				Pesticide losses at 1-m depth (g/ha)			
	OLW	OTW	OLH	OTH	OLW	OTW	OLH	OTH
1985	242	242	224	224	<0.01	<0.01	<0.01	<0.01
1986	241	241	223	223	20.6	<0.01	0.15	<0.01
1987	241	241	223	223	5.17	<0.01	0.16	<0.01
1988	241	241	223	223	<0.01	0.02	<0.01	<0.01
1989	-	241	223	223	-	0.14	<0.01	<0.01
1990	-	241	223	223	-	0.06	<0.01	<0.01
1991	-	241	223	223	-	0.01	<0.01	<0.01
1992	-	241	-	223	-	<0.01	-	<0.01
1993	-	241	-	223	-	<0.01	-	<0.01
1994	-	-	-	223	-	-	-	<0.01

Table 20. Annual percolation and pesticide losses predicted by PELMO for the four scenarios

	OLW	OTW	OLH	OTH
Number of years	4	9	7	10
Total percolation (mm)	963	2166	1565	2235
Total pesticide losses at 1-m depth (g/ha)	25.7	0.23	0.31	1.11×10^{-7}
Total pesticide losses at 1-m depth (% applied)	1.29	0.01	0.02	5.53×10^{-6}

Table 21. Accumulated percolation and pesticide losses predicted by PELMO for the four scenarios

Figure 6 presents monthly pesticide losses predicted by PELMO for the four scenarios. As recharge at the bottom of the soil profile was only predicted to occur from December to April every year, pesticide losses were limited to this period. No major difference was noted in the pesticide breakthrough between the two soils and the compounds. Maximum monthly pesticide loss was predicted to occur after different number of years for the different scenarios (after 2 years for OLW, 4 years for OTW, 3 years for OLH and 5 years for OTH).

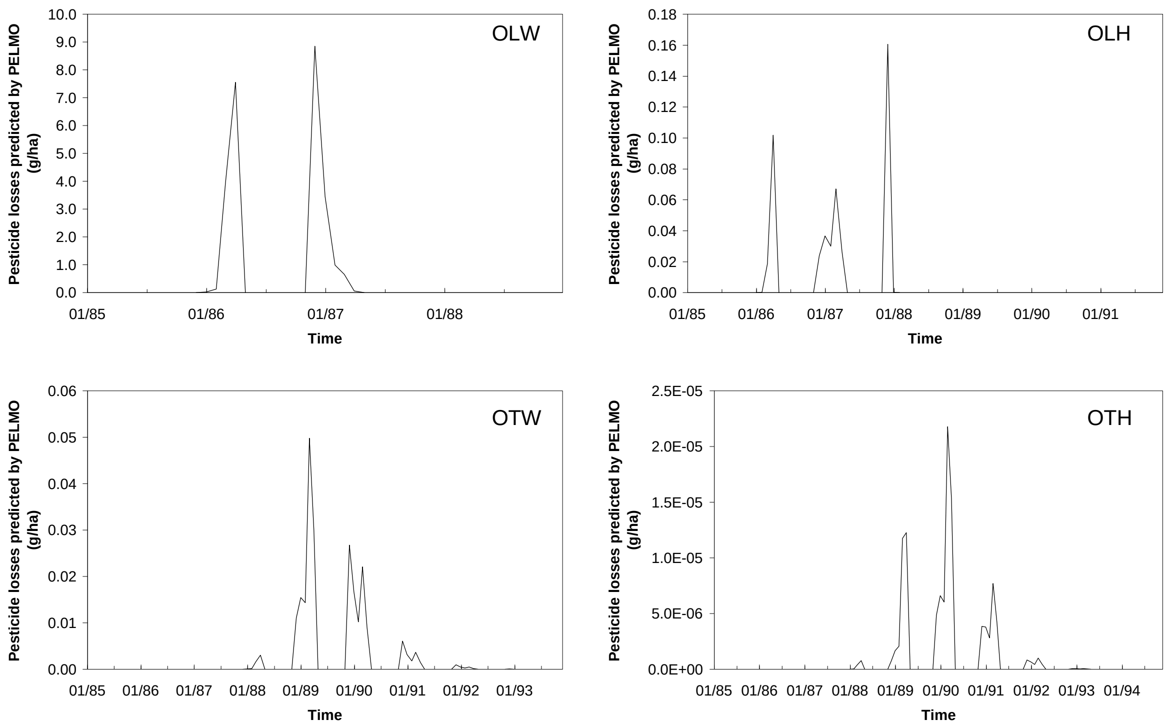

Figure 6. Monthly pesticide losses predicted by PELMO for the four scenarios (g/ha)

3.2.2 Results for the one-at-a-time sensitivity analysis

A total of 944 model runs was carried out to assess the one-at-a-time sensitivity analysis of PELMO to the 18 primary parameters for the four scenarios.

The influence of variation of the parameters on recharge and pesticide losses predicted by PELMO is presented graphically in Appendices 67 to 74 and numerically in Appendices 75 to 82. Examples of charts obtained for Pesticide L in Wick soil are provided in Figures 7 and 8.

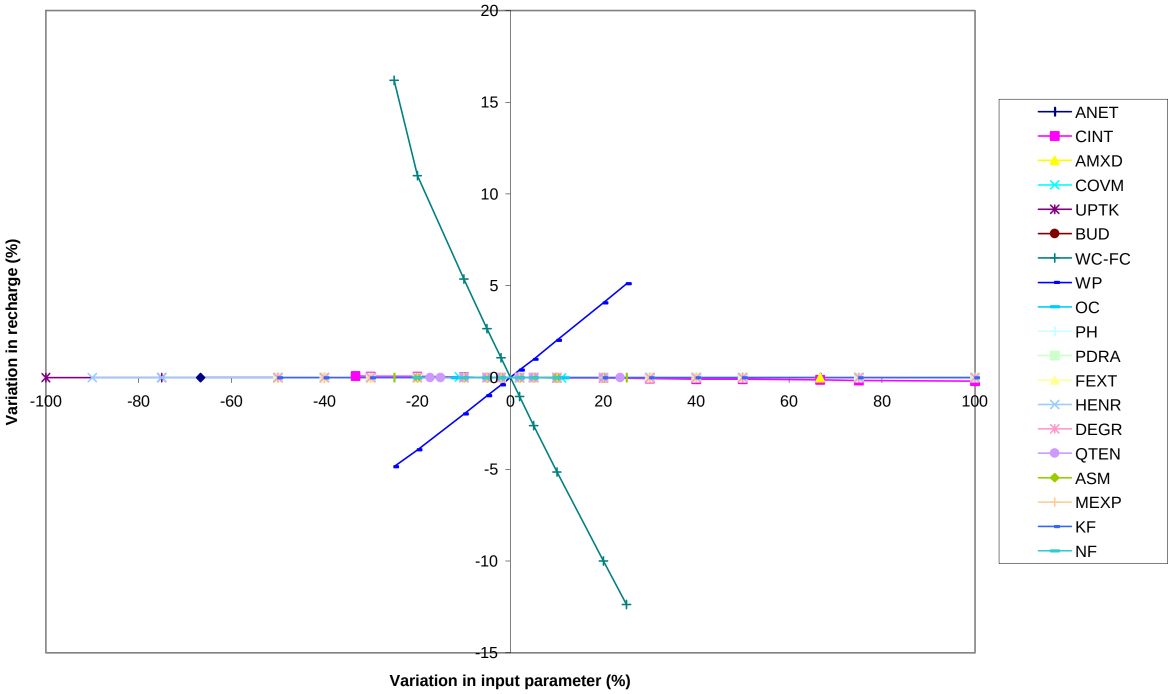

Figure 7. Influence of the variation of input parameters on recharge volumes predicted by PELMO for the OLW (Pesticide L on Wick) scenario

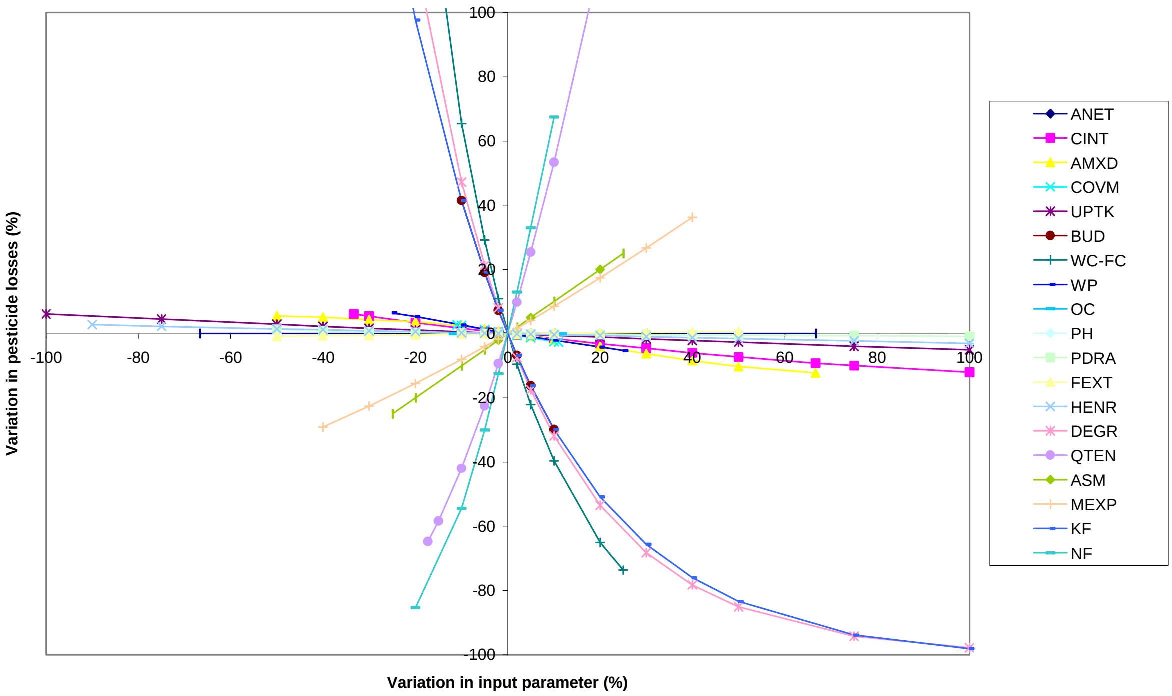

Figure 8. Influence of the variation of input parameters on pesticide losses predicted by PELMO for the OLW (Pesticide L on Wick) scenario

Tables 22 and 23 provide summaries of the sensitivity of the model to changes in input parameters for the four scenarios.

		Wick		Hodnet		
		Pesticide L	Pesticide T	Pesticide L	Pesticide T	Influence
WC-FC	Water capacity – Field capacity	0.648	0.641	1.167	1.165	-
WP	Wilting point	0.208	0.208	0.519	0.519	+
CINT	Maximum interception storage	0.003	0.004	0.019	0.020	-
COVM	Maximum soil cover	0.003	0.004	0.019	0.020	-
ANET	Depth of evapotranspiration computation	0	0	0	0	
AMXD	Maximum active rooting depth	0	0	0	0	
UPTK	Plant uptake efficiency factor	0	0	0	0	
BUD	Bulk density	0	0	0	0	
PDRA	Plant decay rate	0	0	0	0	
FEXT	Foliar extraction coefficient	0	0	0	0	
HENR	Henry's constant	0	0	0	0	
DEGR	Degradation rate	0	0	0	0	
QTEN	Increase given a temperature increase of 10°C	0	0	0	0	
ASM	Soil moisture during degradation	0	0	0	0	
MEXP	Exponent for moisture correction	0	0	0	0	
KF	Freundlich sorption coefficient	0	0	0	0	
NF	Freundlich exponent	0	0	0	0	

Table 22. Classification of PELMO parameters according to their influence on recharge (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase of recharge and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive
Very sensitive
Moderately sensitive
Slightly sensitive
Insensitive

		Wick		Hodnet		
		Pesticide L	Pesticide T	Pesticide L	Pesticide T	Influence
DEGR	Degradation rate	12.345	197.923	110.485	16384.020	-
KF	Freundlich sorption coefficient	7.536	274.312	34.477	14425.139	-
NF	Freundlich exponent	6.746	167.301	36.750	6923.228	+
WC-FC	Water capacity – Field capacity	10.342	37.750	67.764	450.205	-
QTEN	Increase given a temperature increase of 10°C	5.983	22.288	17.262	94.061	+
BUD	Bulk density	4.147	23.175	8.129	46.539	-
ASM	Soil moisture during degradation	3.002	12.230	7.319	31.998	+
MEXP	Exponent for moisture correction	0.906	5.424	1.028	4.160	+
COVM	Maximum soil cover	0.255	0.762	0.376	0.864	-
CINT	Maximum interception storage	0.184	0.730	0.300	0.865	-
WP	Wilting point	0.288 (-)	0.335 (-)	0.683 (-)	0.517 (+)	-/+
AMXD	Maximum active rooting depth	0.375	0.343	0.197	0.331	-
UPTK	Plant uptake efficiency factor	0.061	0.375	0.059	0.355	-
FEXT	Foliar extraction coefficient	0.021	0.046	0.033	0.046	+
PDRA	Plant decay rate	0.026	0.038	0.033	0.039	-
HENR	Henry's constant	0.045	0	0.039	0	-
ANET	Depth of evapotranspiration computation	0	0	0	0	

Table 23. Classification of PELMO parameters according to their influence on pesticide losses (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase of pesticide losses and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive
Very sensitive
Moderately sensitive
Slightly sensitive
Insensitive

Recharge volumes predicted by PELMO were only sensitive to parameters related to the soil water content (*i.e.* field capacity, initial soil moisture content and wilting point) for all scenarios. Crop related parameters which were considered in this study (maximum interception storage and maximum soil cover) had very little effect on predicted volumes of recharge. The sensitivity of recharge was approximately twice as large for the Hodnet scenarios compared to the Wick scenarios.

In contrast to recharge, the prediction of pesticide losses was extremely sensitive (MAROV>10) to some parameters. The maximum MAROV value was >10,000 for the Pesticide T on Hodnet scenario. Such large sensitivities were dismissed on the basis of the small pesticide loss predicted for this particular scenario. It is likely that the sensitivity of PELMO was related to some extent to the amount of pesticide loss that was predicted (the greater the loss, the less sensitive the model), although this was only verified within soil type in this study (sensitivity for OLW < sensitivity for OTW and sensitivity for OLH < sensitivity for OTH). Although absolute values for MAROV can be discarded, the use of their ranking remains valid.

Table 24 presents the PELMO parameters ranked by their influence on pesticide losses for the four scenarios. The very sensitive (MAROV>1) and extremely sensitive (MAROV>10) parameters were identical for the four scenarios. These included all parameters related to degradation (degradation rates DEGR, the factor of increase in degradation when temperature is increased by 10°C QTEN, the soil moisture during the incubation during degradation studies ASM, and the exponent of the equation describing the influence of moisture on degradation MEXP), all parameters related to sorption (the Freundlich exponent NF and the Freundlich coefficient KF) and two soil parameters (the field capacity/initial soil moisture content WC/FC and the bulk density BUD).

The four most influential parameters were degradation rates, the Freundlich coefficient and exponent and the field capacity/initial soil moisture content. Ranking of these parameters was influenced by the properties of the pesticide. Field capacity and initial soil moisture content were the second most sensitive parameters for the scenarios involving pesticide L. Some modellers rely on pedotransfer functions or values for a group of soils (*e.g.* the Dutch Winand Staring soil series) to determine field capacity. Where available, the option of direct measurement should be preferred because pedotransfer functions are only approximations and the use of field capacity for soil groups is not soil-specific. The definition of field capacity with regard to its laboratory determination is not universal and discrepancies exist between countries. In Germany and the US, field capacity is defined as the water content at a pressure of *ca.* -33 kPa, but different pressures are used in other countries (-5 kPa in the UK, -10 kPa in the Netherlands, -6 kPa in Canada). There is no recommendation for the use of a specific pressure in the PELMO manual. Table 24 shows that losses predicted by PELMO can be significantly influenced by field capacity and a small discrepancy in the pressures at which measurement is made may result in large discrepancies in predicted losses. Furthermore, the determination of field capacity is uncertain because of spatial, temporal and analytical variability.

	OLW		OTW		OLH		OTH	
1	DEGR	12.3	KF	274.3	DEGR	110.5	DEGR	16384
2	WC-FC	10.3	DEGR	197.9	WC-FC	67.8	KF	14425
3	KF	7.54	NF	167.3	NF	36.7	NF	6923
4	NF	6.75	WC-FC	37.8	KF	34.5	WC-FC	450
5	QTEN	5.98	BUD	23.2	QTEN	17.3	QTEN	94.1
6	BUD	4.15	QTEN	22.3	BUD	8.13	BUD	46.5
7	ASM	3.00	ASM	12.2	ASM	7.32	ASM	32.0
8	MEXP	0.906	MEXP	5.42	MEXP	1.03	MEXP	4.16
9	AMXD	0.375	COVM	0.760	WP	0.683	CINT	0.865
10	WP	0.288	CINT	0.730	COVM	0.376	COVM	0.864
11	COVM	0.255	UPTK	0.375	CINT	0.300	WP	0.517
12	CINT	0.184	AMXD	0.343	AMXD	0.197	UPTK	0.355
13	UPTK	0.061	WP	0.335	UPTK	0.059	AMXD	0.331
14	HENR	0.045	FEXT	0.046	HENR	0.039	FEXT	0.046
15	PDRA	0.026	PDRA	0.038	FEXT	0.033	PDRA	0.039
16	FEXT	0.021	HENR	0	PDRA	0.033	HENR	0

Table 24. The 15 most influential parameters on the prediction of pesticide losses by PELMO for the four scenarios as determined by one-at-a-time sensitivity analysis (classification by MAROV values)

3.2.3 Results for the Monte Carlo analysis

PELMO input parameters obtained from sampling in the different probability distributions are presented in Appendices 93 to 96. A total of 250 runs were carried out for each scenario using the sampled input parameters. Basic statistics on the percolation and pesticide losses predicted by MACRO are presented in Table 25. More detailed statistics can be found in Appendices 104 to 106.

	Recharge (mm)				Pesticide losses (g/ha)			
	OLW	OTW	OLH	OTH	OLW	OTW	OLH	OTH
Minimum	842.2	1890.0	1212.6	1768.2	0.0	0.0	0.0	0.0
Mean	965.2	2170.4	1583.5	2265.1	59.6	9.3	4.0	0.56
Median	963.5	2164.6	1578.7	2244.5	28.8	0.2	0.4	0.0
Maximum	1127.5	2540.4	2091.1	3007.4	452.7	9.26	63.8	20.1
CV (%)	6	6	10	10	127	279	222	411

Table 25. Basic statistics on PELMO predictions for the four scenarios using input parameters generated by Monte Carlo sampling

Regression techniques were used for non-transformed standardised data and transformed (ranked) standardised data. Coefficients of determination related to pesticide losses for the transformed data (r^2 0.92-0.95) were significantly larger than those for non-transformed data

(r^2 0.25-0.65) because of the inherent non-linearity in the prediction of pesticide losses by PELMO. Classification of parameters according to their influence on prediction of recharge and pesticide losses was therefore conducted using Standardised Rank Regression Coefficients only (Tables 26 and 27). The larger the absolute values of the regression coefficients (SRCC) the more influence the parameter has. An increase in a parameter with a positive SRCC will result in an increase in the model output and vice versa.

	OLW		OTW		OLH		OTH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
WC_FC	-0.9913	1	-0.9812	1	-0.9711	1	-0.9749	1
WP	0.1412	2	0.1369	2	0.2084	2	0.2149	2
PDRA	-0.0023	12	0.0027	12	-0.0007	19	0.0217	3
CINTCP	-0.0082	3	-0.0054	5	-0.0028	14	-0.0080	7
AMXDR	0.0018	16	-0.0057	4	-0.0070	6	0.0093	5
ANETD	-0.0012	17	0.0026	14	-0.0115	3	0.0062	11
FEXT	0.0020	15	0.0068	3	0.0049	11	-0.0075	9
ASM	0.0064	5	0.0011	18	-0.0050	10	-0.0086	6
COVMAX	0.0044	8	-0.0028	11	-0.0018	16	0.0110	4
OC	-0.0055	7	-0.0043	6	0.0072	5	-0.0026	15
UPTK	-0.0042	9	-0.0043	7	0.0025	15	-0.0080	8
KF	-0.0056	6	0.0038	8	0.0059	7	-0.0035	13
BUD	-0.0076	4	-0.0029	10	0.0007	18	-0.0054	12
PH	0.0022	13	-0.0034	9	-0.0074	4	-0.0035	14
MEXP	0.0037	10	-0.0001	19	0.0052	9	0.0072	10
HENR	-0.0034	11	-0.0017	16	-0.0044	12	0.0025	16
NF	-0.0009	18	-0.0017	15	-0.0056	8	0.0010	19
DEGR	-0.0008	19	-0.0027	13	0.0035	13	0.0014	17
QTEN	0.0021	14	0.0015	17	-0.0008	17	0.0012	18

Table 26. Classification of PELMO input parameters according to their influence on results for recharge (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

	OLW		OTW		OLH		OTH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
DEGR	-0.6316	1	-0.4369	3	-0.5302	1	-0.4251	3
KF	-0.5054	2	-0.5632	1	-0.4609	2	-0.4639	2
NF	0.2400	5	0.5628	2	0.4119	3	0.6755	1
WC_FC	-0.2931	3	-0.2111	4	-0.3158	4	-0.1697	4
QTEN	0.2860	4	0.1523	5	0.2502	5	0.1458	5
ASM	0.1648	6	0.1007	7	0.1296	6	0.1027	6
BUD	-0.1028	7	-0.0811	8	-0.0661	7	-0.0420	8
MEXP	0.0667	8	0.1038	6	0.0300	9	0.0326	9
AMXDR	-0.0363	9	-0.0603	9	-0.0177	10	-0.0284	10
FEXT	0.0256	11	-0.0175	12	-0.0067	18	-0.0500	7
WP	0.0176	12	-0.0441	10	0.0094	15	0.0019	19
CINTCP	-0.0287	10	0.0076	16	-0.0106	14	-0.0152	12
ANETD	-0.0016	18	0.0010	19	-0.0370	8	-0.0085	14
UPTK	0.0128	13	0.0089	14	-0.0131	12	-0.0126	13
HENR	-0.0115	15	-0.0072	17	0.0048	19	0.0193	11
COVMAX	0.0127	14	-0.0078	15	0.0144	11	-0.0062	15
PH	0.0006	19	-0.0224	11	-0.0093	16	0.0056	17
OC	0.0067	16	-0.0156	13	0.0070	17	-0.0056	16
PDRA	-0.0060	17	0.0048	18	-0.0113	13	0.0033	18

Table 27. Classification of PELMO input parameters according to their influence on results for pesticide losses (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

Table 26 shows that recharge volumes are almost exclusively sensitive to the parameters WC (soil moisture content at the beginning of the simulation period) and FC (soil moisture content at field capacity) which were linked in this study. The sensitivity of recharge predicted by PELMO can therefore be estimated using a simple linear regression. However, it is likely that the effects of these two parameters will be overruled by the importance of the difference between rainfall and potential evapotranspiration (PET). Measured rainfall and calculated PET are uncertain variables. Uncertainty in rainfall data mainly originates from experimental inaccuracies in the measurement of precipitation. Uncertainty in PET results from the existence of different formulas for calculating PET which lead to different PET estimations. Recommendations for the calculation of PET to be used in pesticide fate models should be derived. Also, the different treatment of PET by different models to derive actual evapotranspiration should be addressed.

Most of the PELMO input parameters which were varied did not have any influence on prediction of recharge, as showed in the one-at-a-time sensitivity analysis. These were nevertheless attributed a regression coefficient when using linear regression techniques (Table 26). For instance, the pesticide degradation rate (PDRA) was rated the third most influential parameter on the prediction of recharge in the OTH scenario, but the importance given to this parameter is obviously flawed. It is therefore recommended that the use of linear regression techniques and Monte Carlo sampling is limited to parameters that are known to have an influence of the output under investigation. This may require a limited one-at-a-time sensitivity analysis to be carried out.

Table 27 shows a ranking of PELMO parameters according to their influence on the prediction of pesticide losses. Predictions for pesticide losses were largely influenced by parameters related to sorption and degradation and by the water content at field capacity, to a lesser extent. Regression coefficients were well below unity and 6-7 parameters presented a SRCC >0.1. This stresses the more complex description of pesticide fate in PELMO as compared to the description of water flow phenomena.

	OLW		OTW		OLH		OTH	
1	DEGR	-0.632	KF	-0.563	DEGR	-0.530	NF	0.675
2	KF	-0.505	NF	0.563	KF	-0.461	KF	-0.464
3	WC_FC	-0.293	DEGR	-0.437	NF	0.412	DEGR	-0.425
4	QTEN	0.286	WC_FC	-0.211	WC_FC	-0.316	WC_FC	-0.170
5	NF	0.240	QTEN	0.152	QTEN	0.250	QTEN	0.146
6	ASM	0.165	MEXP	0.104	ASM	0.130	ASM	0.103
7	BUD	-0.103	ASM	0.101	BUD	-0.066	FEXT	-0.050
8	MEXP	0.067	BUD	-0.081	ANET	-0.037	BUD	-0.042
9	AMXD	-0.036	AMXD	-0.060	MEXP	0.030	MEXP	0.033
10	CINT	-0.029	WP	-0.044	AMXD	-0.018	AMXD	-0.028
11	FEXT	0.026	PH	-0.022	COVM	0.014	HENR	0.019
12	WP	0.018	FEXT	-0.017	UPTK	-0.013	CINT	-0.015
13	UPTK	0.013	OC	-0.016	PDRA	-0.011	UPTK	-0.013
14	COVM	0.013	UPTK	0.009	CINT	-0.011	ANET	-0.009
15	HENR	-0.012	COVM	-0.008	WP	0.009	COVM	-0.006

Table 28. The 15 most influential parameters on the prediction of pesticide losses by PELMO for the four scenarios (Monte Carlo sampling).
Parameters are classified according by Standardised Rank Regression Coefficients (SRRC).

3.3 PRZM 3.14b

3.3.1 Results for the four scenarios (the four "base-cases")

Tables 29 and 30 present annual and cumulative water percolation and pesticide losses simulated by PRZM for the four scenarios. Predicted percolation was very similar for the Hodnet and Wick soils (mean annual difference 12 mm). It is not clear why annual values for percolation for non-leap years were predicted to be different as the same weather data were used for each of the 10 years of simulation. Total pesticide losses were predicted to be largest for the Pesticide L on Wick scenario (31.7 g/ha). Virtually no pesticide leaching was predicted for the scenario describing the leaching of pesticide T in the Hodnet soil. Pesticide losses were predicted to be larger for pesticide L than for pesticide T for a given soil. Also, larger losses were predicted by PRZM from the sandy loam Wick soil than from the more structured Hodnet soil. These findings are similar to those reported for PELMO.

	Percolation (mm)				Pesticide losses at 1-m depth (g/ha)			
	ZLW	ZTW	ZLH	ZTH	ZLW	ZTW	ZLH	ZTH
1985	350	350	347	347	0.03	<0.01	<0.01	<0.01
1986	305	305	293	293	28.8	<0.01	0.67	<0.01
1987	305	305	293	293	2.85	<0.01	0.22	<0.01
1988	306	306	294	294	<0.01	0.09	<0.01	<0.01
1989	305	305	293	293	<0.01	0.24	<0.01	<0.01
1990	305	305	293	293	<0.01	0.14	<0.01	<0.01
1991	305	305	293	293	<0.01	0.03	<0.01	<0.01
1992	297	297	281	281	<0.01	<0.01	<0.01	<0.01
1993	297	297	280	280	<0.01	<0.01	<0.01	<0.01
1994	297	297	280	280	<0.01	<0.01	<0.01	<0.01

Table 29. Annual percolation and pesticide losses predicted by PRZM for the four scenarios

	ZLW	ZTW	ZLH	ZTH
Number of years	10	10	10	10
Total percolation (mm)	3071	3071	2948	2948
Total pesticide losses at 1-m depth (g/ha)	31.7	0.52	0.89	4.04×10^{-3}
Total pesticide losses at 1-m depth (% applied)	1.59	0.03	0.04	2.02×10^{-4}

Table 30. Accumulated percolation and pesticide losses predicted by PRZM for the four scenarios

Figure 9 presents monthly pesticide losses predicted by PRZM for the four scenarios. No major pesticide leaching was predicted between May and September of each year since PRZM did not predict that water would leach out of the bottom of the soil cores. Pesticide leaching profiles were similar for the two soils, but differed significantly between the two pesticides. Pesticide L was characterised by a leaching pattern which started at the end of the first year and which extended over two years, whereas leaching for pesticide T was initiated later (*i.e.* end of the third year) and lasted for five years.

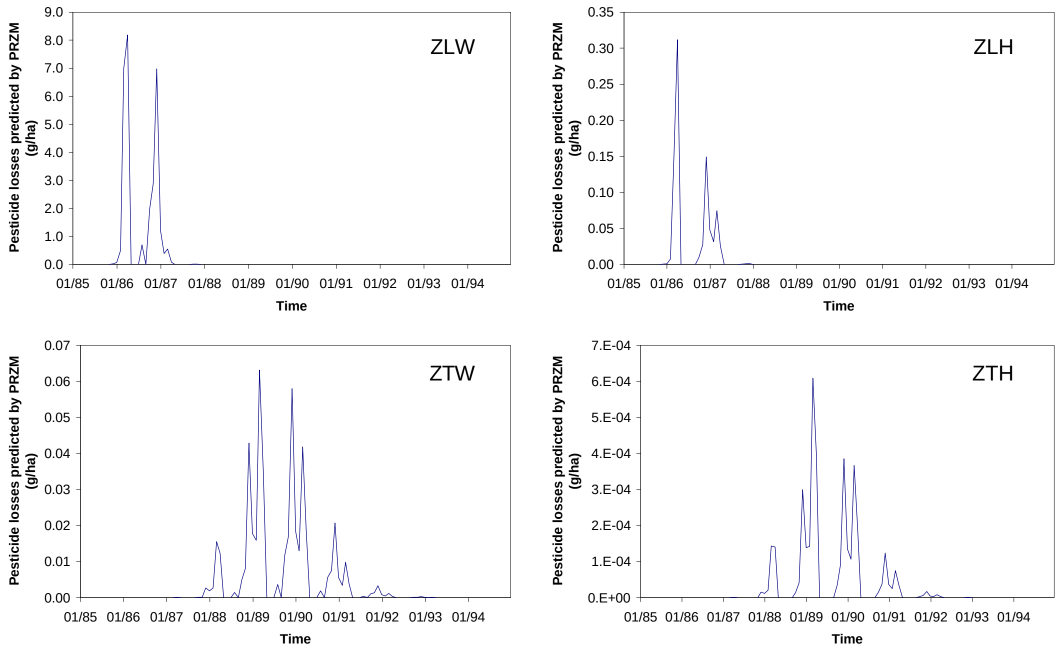

Figure 9. Monthly pesticide losses predicted by PRZM for the four scenarios (g/ha)

3.3.2 Results for the one-at-a-time sensitivity analysis

A total of 952 runs was carried out to assess the sensitivity of PRZM to the 22 primary parameters for the four scenarios, using the one-at-a-time approach.

The influence of variation of the parameters on the prediction of recharge and pesticide losses by PRZM is presented graphically in Appendices 123 to 130 and numerically in Appendices 131 to 138. Examples of charts obtained for Pesticide L in the Wick soil are provided in Figures 10 and 11.

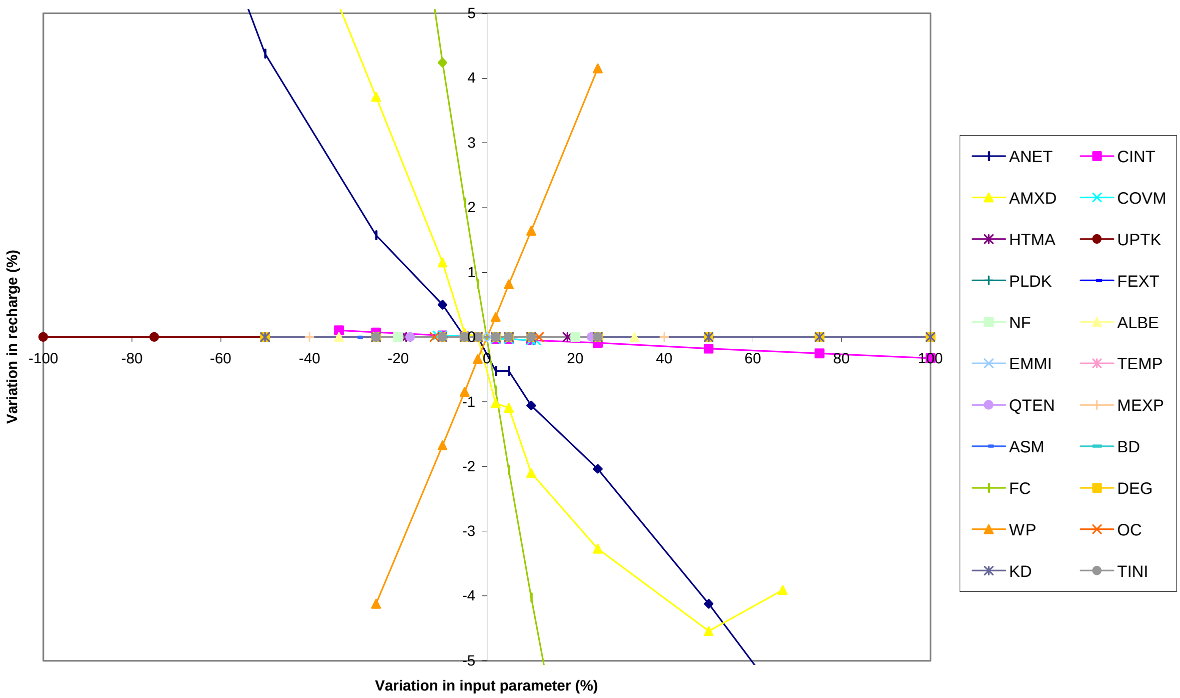

Figure 10. Influence of the variation of input parameters on recharge volumes predicted by PRZM for the ZLW (Pesticide L on Wick) scenario

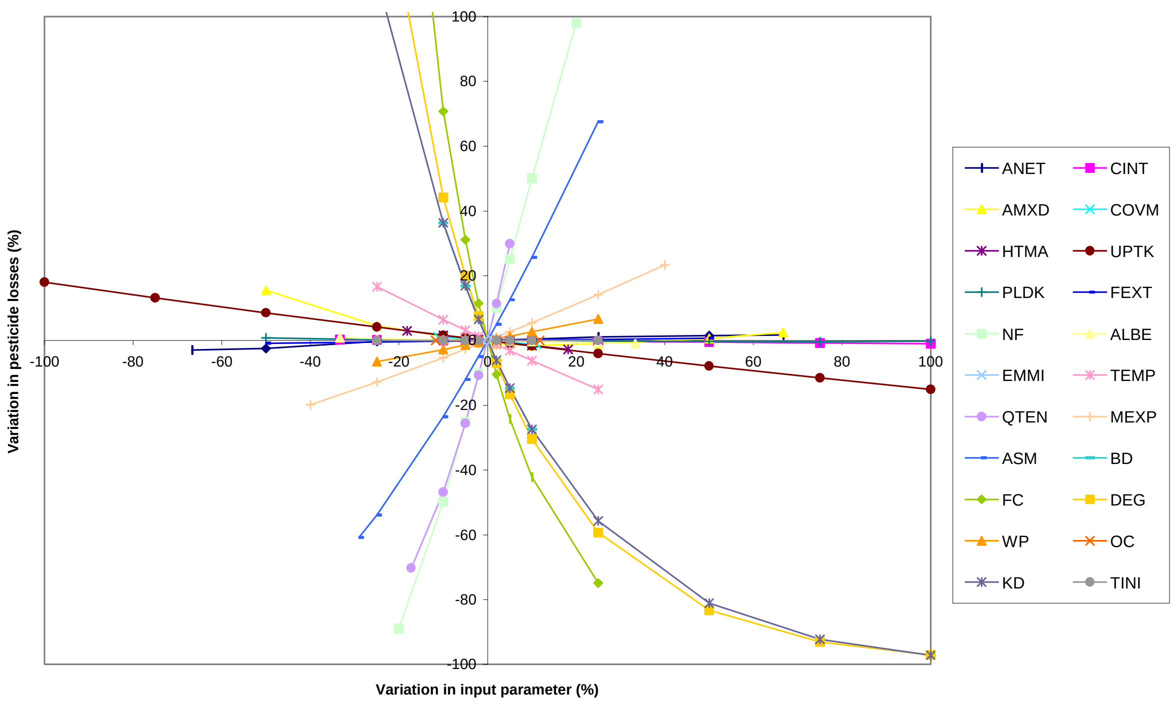

Figure 11. Influence of the variation of input parameters on pesticide losses predicted by PRZM for the ZLW (Pesticide L on Wick) scenario

Tables 31 and 32 provide summaries of the sensitivity of the model to changes in input parameters for the four scenarios.

		Wick		Hodnet		
		Pesticide L	Pesticide T	Pesticide L	Pesticide T	Influence
FC	Field Capacity	0.457	0.457	0.613	0.613	-
ANET	Min. depth for extraction of evap.	0.262	0.262	0.290	0.290	-
WP	Wilting point	0.169	0.169	0.324	0.324	+
AMXD	Maximum rooting depth	0.210	0.210	0.235	0.235	-
CINT	Maximum interception storage	0.015	0.015	0.015	0.015	-
COVM	Maximum areal coverage of canopy	0.015	0.015	0.015	0.015	-
HTMA	Maximum canopy height	0	0	0	0	
UPTK	Plant uptake factor	0	0	0	0	
PLDK	Pesticide decay rate on canopy	0	0	0	0	
FEXT	Foliar extraction coefficient	0	0	0	0	
NF	Freundlich exponent	0	0	0	0	
A	Albedo	0	0	0	0	
EM	Emmissivity	0	0	0	0	
T	Average monthly temp at BB	0	0	0	0	
QTEN	qten	0	0	0	0	
MEXP	Moisture exponent for degradation	0	0	0	0	
ASM	Reference moisture for degradation	0	0	0	0	
BD	Bulk density	0	0	0	0	
DEG	Degradation rate	0	0	0	0	
OC	Organic carbon content	0	0	0	0	
KD	Freundlich coefficient	0	0	0	0	
TINI	Initial temp of the horizon	0	0	0	0	

Table 31. Classification of PRZM parameters according to their influence on recharge (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase of recharge and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive
Very sensitive
Moderately sensitive
Slightly sensitive
Insensitive

		Wick		Hodnet		
		Pesticide L	Pesticide T	Pesticide L	Pesticide T	Influence
NF	Freundlich exponent	5.1	182.1	21.2	3476.9	+
KD	Freundlich coefficient	6.1	204.6	16.9	1061.1	-
DEG	Degradation rate	11.1	138.9	59.7	1061.9	-
QTEN	qten	7.4	35.6	18.9	91.4	+
FC	Field Capacity	11.4	43.5	18.6	33.8	-
BD	Bulk density	3.6	17.6	6.1	21.9	-
ASM	Reference moisture for degradation	2.7	9.9	5.6	18.8	+
T	Average monthly temp at BB	0.663	1.8	1.7	4.1	-
MEXP	Moisture exponent for degradation	0.583	2.6	0.234	1.1	+
WP	Wilting point	0.282	0.430	0.618	2.0	+
ANET	Min. depth for extraction of evap.	0.099 (+)	0.488 (+/-)	0.043 (+/-)	1.8 (-)	+/-
EM	Emmissivity	0.284	0.753	0.393	0.929	+
AMXD	Maximum rooting depth	0.533 (+/-)	0.649 (+/-)	0.496 (+/-)	0.359 (+/-)	+/-
HTMA	Maximum canopy height	0.164	0.401	0.237	0.485	-
UPTK	Plant uptake factor	0.180	0.279	0.206	0.295	-
PLDK	Pesticide decay rate on canopy	0.017 (-)	0.177 (-)	0.114 (+)	0.613 (-)	+/-
COVM	Maximum areal coverage of canopy	0.114	0.230	0.137	0.266	-
FEXT	Foliar extraction coefficient	0.019 (+)	0.072 (+/-)	0.039 (+)	0.306 (+/-)	+/-
A	Albedo	0.035	0.102	0.050	0.126	-
CINT	Maximum interception storage	0.013	0.056	0.028	0.088	-
OC	Organic carbon content	0	0	0	0	
TINI	Initial temp of the horizon	0	0	0	0	

Table 32. Classification of PRZM parameters according to their influence on pesticide losses (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase of pesticide losses and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive
Very sensitive
Moderately sensitive
Slightly sensitive
Insensitive

Results from the sensitivity analysis with regard to the prediction of recharge by PRZM were only dependent on the soil considered and not on the pesticide. For both soils, recharge volumes predicted by PRZM were only sensitive to a few parameters. The magnitude of the change in predicted recharge was rather small (MAROV<0.7) and it was only marginally affected by the nature of the soil. The input parameter which had the most influence on predictions was "field capacity", which consists in the field capacity value as determined from the water release curve and the soil moisture content at the beginning of the simulations (*i.e.* initial soil moisture content was set at field capacity). Other parameters which were found to influence the prediction of recharge were those related to the moisture status of the soil (wilting point), to the computation of the actual evapotranspiration from potential evapotranspiration data (minimum depth for extraction of evaporation) and to the description of the plant cover (maximum rooting depth, maximum interception storage and maximum areal coverage of the canopy).

In contrast to the prediction of recharge volumes, prediction of losses of pesticides by PRZM were very much affected by changes in input parameters. The magnitude of the sensitivities changed according to the different scenarios. Large to very large sensitivities were found for all four scenarios (maximum MAROV value ~3500) and the largest sensitivities were attributed to pesticide T which leached only to a small extent in both soils.

Table 33 presents the 15 parameters which were found to most influence predictions of total pesticide losses by PRZM. Although the most influential parameters were different for each scenario, the same parameters were consistently found at the top of the list. This is particularly obvious for the first six parameters at the top of the table, which are related to pesticide sorption (Freundlich distribution coefficients and exponent), pesticide degradation (degradation rates, QTEN) as well as the description of the soil (field capacity/initial soil moisture content, bulk density). Field capacity appeared as one of the most influential parameters for predictions of pesticide losses by PRZM (see for instance scenario involving Pesticide L in the Wick soil). Again, there is some uncertainty in PRZM as to how the field capacity should be calculated as rules for deriving field capacity values vary between countries.

The organic carbon content was not found to have any influence on prediction of pesticide losses (Table 32) because Kd values were used directly in the input file. Nevertheless, it should be noted that variation in organic carbon would have significantly influenced PRZM predictions if the Koc approach (*i.e.* supplying the Koc and organic carbon content for each soil horizon) had been used. The initial temperature of the different layers of the soil profile did not influence PRZM predictions for losses for the four scenarios considered here.

	ZLW		ZTW		ZLH		ZTH	
1	FC	11.4	KD	204.6	DEG	59.7	NF	3476.9
2	DEG	11.1	NF	182.1	NF	21.2	DEG	1061.9
3	QTEN	7.4	DEG	138.9	QTEN	18.9	KD	1061.1
4	KD	6.1	FC	43.5	FC	18.6	QTEN	91.4
5	NF	5.1	QTEN	35.6	KD	16.9	FC	33.8
6	BD	3.6	BD	17.6	BD	6.1	BD	21.9
7	ASM	2.7	ASM	9.9	ASM	5.6	ASM	18.8
8	T	0.663	MEXP	2.6	T	1.7	T	4.1
9	MEXP	0.583	T	1.848	WP	0.618	WP	2.0
10	AMXD	0.533	EM	0.753	AMXD	0.496	ANET	1.8
11	EM	0.284	AMXD	0.649	EM	0.393	MEXP	1.1
12	WP	0.282	ANET	0.488	HTMA	0.237	EM	0.929
13	UPTK	0.180	WP	0.430	MEXP	0.234	PLDK	0.613
14	HTMA	0.164	HTMA	0.401	UPTK	0.206	HTMA	0.485
15	COVM	0.114	UPTK	0.279	COVM	0.137	AMXD	0.359

Table 33. The 15 most influential parameters on the prediction of pesticide losses by PRZM for the four scenarios as determined by one-at-a-time sensitivity analysis (classification by MAROV values)

3.3.3 Results for the Monte Carlo analysis

Descriptive statistics on the values for the PRZM input parameters obtained via sampling into probability distribution functions are presented in Appendices 149 to 152. A total of 250 runs was carried out for each scenario using the randomly sampled values. Basic statistics on the recharge volumes and pesticide losses predicted by PRZM are presented in Table 34. More detailed statistics can be found in Appendices 153 to 162.

	Recharge (mm)				Pesticide losses (g/ha)			
	ZLW	ZTW	ZLH	ZTH	ZLW	ZTW	ZLH	ZTH
Minimum	2584	2642	2419	2435	6.8×10^{-7}	0	3.6×10^{-15}	0
Mean	3075	3075	2943	2943	75.8	19.7	5.2	2.2
Median	3065	3080	2960	2937	40.5	1.1	1.3	0.01
Maximum	3636	3632	3459	3520	468.9	375.6	86.2	63
CV (%)	0.06	0.07	0.07	0.06	1.2	2.4	1.8	3.5

Table 34. Basic statistics on PRZM predictions for the four scenarios

Regression techniques were used for non-transformed standardised data and transformed (ranked) standardised data. Coefficients of determination related to pesticide losses for the transformed data (r^2 0.93-0.96) were significantly larger than those for non-transformed data (r^2 0.34-0.71) because of the inherent non-linearity in the prediction of pesticide losses by PRZM. Classification of parameters according to their influence on prediction of recharge and pesticide losses was therefore conducted using Standardised Rank Regression Coefficients only (Tables 35 and 36). The larger the absolute values of the regression coefficients (SRCC) the more influence the parameter has. An increase in a parameter with a positive SRCC will result in an increase in the model output and vice versa.

	ZLW		ZTW		ZLH		ZTH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
FC	-0.735	1	-0.757	1	-0.561	1	-0.628	1
AMXD	-0.487	2	-0.418	2	-0.469	2	-0.533	2
ANET	-0.373	3	-0.343	3	-0.359	4	-0.409	4
WP	0.275	4	0.278	4	0.438	3	0.462	3
CINT	-0.034	6	0.020	8	-0.031	5	0.032	6
OC	-0.028	7	-0.015	10	0.015	11	-0.031	8
EM	-0.022	9	-0.013	11	-0.015	10	-0.032	7
T	-0.036	5	0.006	20	0.003	19	0.028	9
DEG	-0.009	16	-0.009	16	0.026	6	0.025	10
MEXP	0.014	14	-0.008	18	-0.020	8	0.023	11
KD	0.008	18	0.025	6	0.026	7	0.005	18
PLDK	0.003	20	0.009	14	0.005	18	-0.037	5
BD	0.003	21	-0.022	7	0.018	9	0.010	14
QTEN	0.004	19	-0.027	5	-0.002	21	-0.018	12
ASM	-0.028	8	-0.007	19	-0.010	13	-0.006	16
COVM	-0.020	10	0.017	9	-0.010	12	-0.002	20
HTMA	0.016	12	0.005	21	-0.003	20	-0.016	13
FEXT	0.016	11	-0.009	15	0.009	14	-0.001	22
A	-0.010	15	0.010	12	0.008	15	-0.005	17
TINI	0.009	17	0.008	17	-0.007	17	-0.007	15
UPTK	0.015	13	0.002	22	0.008	16	-0.004	19
NF	0.002	22	-0.010	13	0.001	22	-0.002	21

Table 35. Classification of PRZM input parameters according to their influence on results for recharge (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

	ZLW		ZTW		ZLH		ZTH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
DEG	-0.590	1	-0.450	3	-0.639	1	-0.430	3
KD	-0.523	2	-0.547	1	-0.479	2	-0.451	2
NF	0.243	5	0.523	2	0.462	3	0.684	1
FC	-0.363	3	-0.219	4	-0.264	5	-0.122	5
QTEN	0.278	4	0.207	5	0.280	4	0.197	4
ASM	0.184	6	0.129	6	0.086	6	0.055	6
BD	-0.059	8	-0.091	7	-0.079	7	-0.047	7
MEXP	0.058	9	0.024	11	0.057	8	0.031	9
T	-0.030	10	-0.041	8	-0.056	9	-0.044	8
UPTK	-0.070	7	-0.011	16	-0.054	10	-0.023	10
TINI	0.024	13	0.009	19	0.053	11	0.015	17
AMXD	-0.025	12	-0.014	15	-0.019	17	0.022	11
ANET	0.006	16	-0.010	17	-0.031	12	-0.021	13
EM	0.023	14	-0.018	13	-0.004	19	-0.021	12
WP	0.028	11	0.026	9	-0.003	21	0.003	21
A	0.008	15	-0.001	22	0.028	13	0.018	15
FEXT	-0.001	22	0.008	20	-0.025	15	0.015	16
COVM	-0.006	17	-0.025	10	0.004	20	0.012	18
HTMA	-0.002	20	-0.020	12	-0.007	18	0.012	19
PLDK	0.001	21	-0.016	14	0.020	16	0.003	20
CINT	-0.004	18	-0.002	21	0.026	14	-0.002	22
OC	0.003	19	0.010	18	0.002	22	0.019	14

Table 36. Classification of PRZM input parameters according to their influence on results for pesticide losses (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

Table 35 shows that only the four most sensitive parameters were consistent between the four different scenarios and contributed significantly to the sensitivity of recharge predictions (|SRCC|>0.1). This was expected to some extent since the one-at-a-time sensitivity analysis demonstrated that only six parameters from those selected for this study influenced the prediction of recharge by PRZM. The most influential parameter was the field capacity which had a negative influence on the prediction of recharge (*i.e.* the smaller the field capacity, the more recharge). The next three most sensitive parameters were the maximum rooting depth (AMXD), the minimum depth for extraction of evaporation (ANET) and the wilting point (WP). Results for the Monte Carlo analysis are therefore consistent with those for the one-at-a-time sensitivity analysis for the first few most sensitive parameters. Most of the input parameters did not have any influence on the prediction of recharge volumes as demonstrated in the one-at-a-time sensitivity analysis, but were nevertheless attributed a sensitivity coefficient. Again, this is one of the disadvantages of using an approach that uses a combination of Monte Carlo sampling and multiple linear regressions.

Table 37 presents the 15 parameters which most influence the prediction of pesticide losses by PRZM. Results were fairly consistent with those from the one-at-a-time sensitivity analysis in that the top of the list of the most sensitive parameters was affected by the scenario considered. The most sensitive parameters were those related to the sorption and degradation of pesticides (*i.e.* degradation rates, Freundlich coefficient and exponent). Field capacity was again found to significantly influence prediction of pesticide losses by PRZM, although this was less clear than for the one-at-a-time approach where field capacity was the most sensitive parameter for the ZLW scenario.

	ZLW		ZTW		ZLH		ZTH	
1	DEG	-0.590	KD	-0.547	DEG	-0.639	NF	0.684
2	KD	-0.523	NF	0.523	KD	-0.479	KD	-0.451
3	FC	-0.363	DEG	-0.450	NF	0.462	DEG	-0.430
4	QTEN	0.278	FC	-0.219	QTEN	0.280	QTEN	0.197
5	NF	0.243	QTEN	0.207	FC	-0.264	FC	-0.122
6	ASM	0.184	ASM	0.129	ASM	0.086	ASM	0.055
7	UPTK	-0.070	BD	-0.091	BD	-0.079	BD	-0.047
8	BD	-0.059	T	-0.041	MEXP	0.057	T	-0.044
9	MEXP	0.058	WP	0.026	T	-0.056	MEXP	0.031
10	T	-0.030	COVM	-0.025	UPTK	-0.054	UPTK	-0.023
11	WP	0.028	MEXP	0.024	TINI	0.053	AMXD	0.022
12	AMXD	-0.025	HTMA	-0.020	ANET	-0.031	ANET	-0.021
13	TINI	0.024	EM	-0.018	A	0.028	EM	-0.021
14	EM	0.023	PLDK	-0.016	CINT	0.026	OC	0.019
15	A	0.008	AMXD	-0.014	FEXT	-0.025	A	0.018

Table 37. The 15 most influential parameters on the prediction of pesticide losses by PRZM for the four scenarios (Monte Carlo sampling).

3.4 PESTLA 3.4

3.4.1 Results for the four scenarios (the four "base-cases")

Tables 38 and 39 present annual and cumulative percolation and losses of pesticide simulated by PESTLA for the four scenarios. Predicted water percolation was similar for the two soil scenarios (annual difference 3 mm). Total pesticide losses were predicted to be 38.8 g/ha for the scenario involving Pesticide L in the Wick soil, but predictions were much smaller for the three remaining scenarios. Virtually no leaching was predicted for the scenario involving Pesticide T and Hodnet soil (total losses 0.043 g/ha). Losses were predicted to be larger for pesticide L than for pesticide T. For a given pesticide, pesticide losses were predicted to be larger in the sandy loam than in the more structured clay loam. This is partly due to the non-inclusion of a description of preferential flow processes in PESTLA.

	Percolation (mm)				Pesticide losses at 1-m depth (g/ha)			
	ALW	ATW	ALH	ATH	ALW	ATW	ALH	ATH
1985	326	326	329	329	<0.01	0	<0.01	0
1986	326	326	329	329	38.50	<0.01	3.22	<0.01
1987	326	326	329	329	0.30	0.34	0.04	0.03
1988	326	326	329	329	0	0.24	0	0.02
1989	326	326	329	329	0	<0.01	0	<0.01
1990	326	326	329	329	0	<0.01	0	0
1991	326	326	329	329	0	0	0	0
1992	326	326	329	329	0	0	0	0

Table 38. Annual percolation and pesticide losses predicted by PESTLA for the four scenarios

	ALW	ATW	ALH	ATH
Number of years	8	8	8	8
Total percolation (mm)	2608	2608	2632	2632
Total pesticide losses at 1-m depth (g/ha)	38.800	0.606	3.260	0.043
Total pesticide losses at 1-m depth (% applied)	1.84	0.03	0.16	2.1×10^{-3}

Table 39. Accumulated percolation and pesticide losses predicted by PESTLA for the four scenarios

Figure 12 presents daily pesticide losses predicted by PESTLA for the four scenarios. Leaching breakthrough appeared to be dependent on the compound considered. For pesticide L (scenarios ALW and ALH), losses by percolation occurred over a period of one year, whereas losses were simulated over three to four years for Pesticide T. Losses for pesticide L were dominated by a single leaching event occurring in mid-April 1986, whereas losses for pesticide T were more evenly distributed between the years.

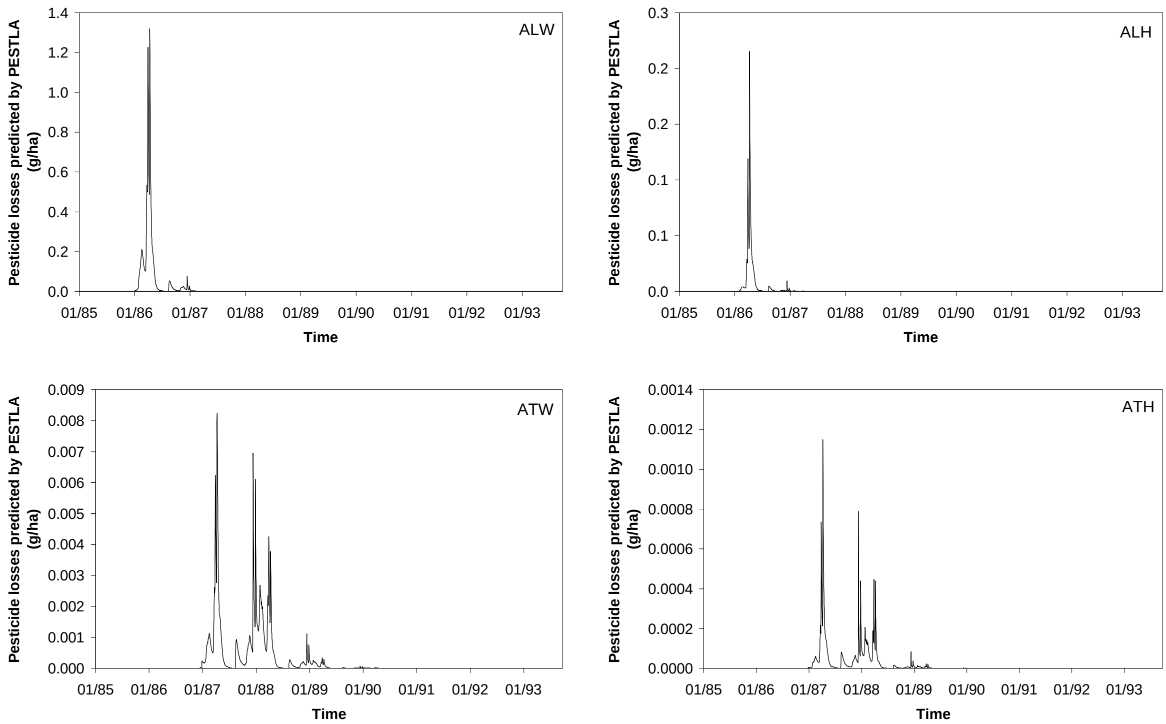

Figure 12. Daily pesticide losses predicted by PESTLA for the four scenarios (g/ha)

3.4.2 Results for the one-at-a-time sensitivity analysis

A total of 1408 model runs were carried out to assess the one-at-a-time sensitivity of PESTLA to the 34 primary parameters for the four scenarios.

The results of the influence of input parameters on the prediction of percolation and pesticide losses are presented graphically in Appendices 188 to 195. Examples of charts for the ALW scenario are presented in Figures 13 and 14. These charts present the variation in PESTLA output (either cumulative percolation or cumulative pesticide losses) vs. the variation in the input.

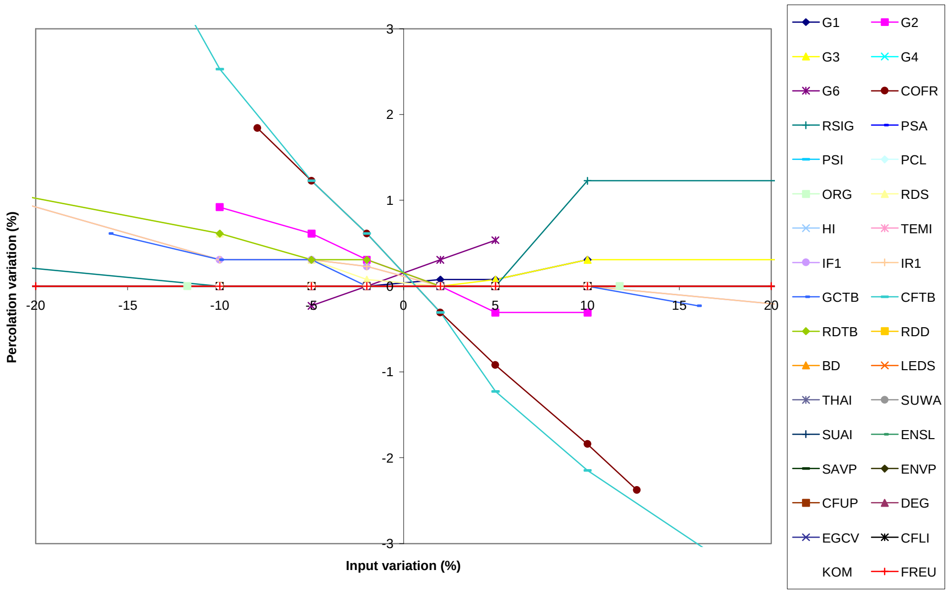

Figure 13. Influence of the variation of input parameters on recharge volumes predicted by PESTLA for the ALW (Pesticide L on Wick) scenario

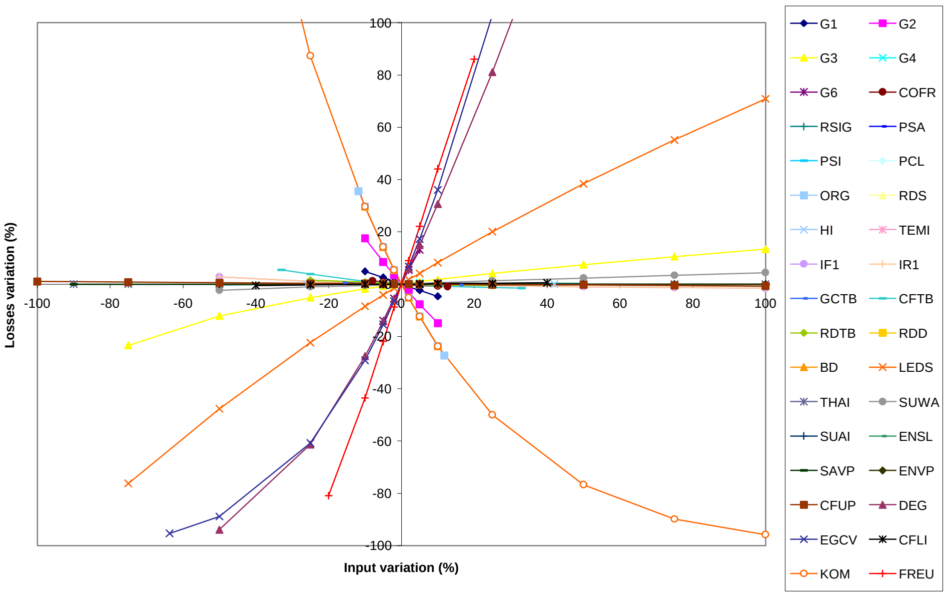

Figure 14. Influence of the variation of input parameters on pesticide losses predicted by PESTLA for the ALW (Pesticide L on Wick) scenario

Table 40 and 41 provide summaries of the sensitivity of the model to changes in input parameters for the four scenarios.

		Wick		Hodnet		
		Pesticide L	Pesticide T	Pesticide L	Pesticide T	Influence
CFTB	Crop factor	0.331	0.331	0.332	0.332	-
COFR	Soil evaporation coefficient of Blak and Boesten or Boesten/Stroosnijder	0.307	0.307	0.304	0.304	-
G6	Parameter n	0.153	0.153	0.243	0.243	+
RSIG	Minimum rainfall to reset models	0.123	0.123	0.134	0.134	+/-
IF1	Extinction coefficient for diffuse visible light	0.115	0.115	0.061	0.061	-
IR1	Extinction coefficient for direct visible light	0.115	0.115	0.061	0.061	-
G2	Saturated moisture content	0.153	0.153	0	0	-
RDTB	maximum rooting depth	0.153	0.153	0	0	-
GCTB	Maximum leaf area index	0.061	0.061	0.030	0.030	-
RDS	maximum rooting depth allowed by soil profile	0.061	0.061	0	0	-
G1	Residual moisture content	0.038	0.038	0	0	+
G3	Saturated hydraulic conductivity	0.031	0.031	0.004	0.004	+
G4	Alpha main drying curve	0	0	0.015	0.015	-
PSA	sand content	0	0	0	0	
PSI	silt content	0	0	0	0	
PCL	clay content	0	0	0	0	
ORG	organic matter content	0	0	0	0	
HI	initial pressure heads	0	0	0	0	
TEMI	initial soil temperatures	0	0	0	0	
RDD	Root density distribution	0	0	0	0	
BD	Bulk density	0	0	0	0	
LEDS	Lengths of dispersion in liquid phase	0	0	0	0	
THAI	Thickness of the stagnant air layer at soil surface	0	0	0	0	
SUWA	Coefficient of diffusion in water	0	0	0	0	
SUAI	Coefficient of diffusion in air	0	0	0	0	
ENSL	Molar enthalpy of the dissolution process	0	0	0	0	
SAVP	Saturated vapour pressure	0	0	0	0	
ENVP	Molar enthalpy of the vaporisation process	0	0	0	0	
CFUP	Coefficient of uptake by plants	0	0	0	0	
DEG	Half life	0	0	0	0	
EGCV	Molar activation energy of degradation	0	0	0	0	
CFLI	Coefficient describing the relationship between the conversion rate and the volume fraction of liquid	0	0	0	0	
KOM	Kom	0	0	0	0	
FREU	Freundlich exponent	0	0	0	0	

Table 40. Classification of PESTLA parameters according to their influence on recharge (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase of recharge and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive	Slightly sensitive
Very sensitive	Insensitive
Moderately sensitive	

		Wick		Hodnet		
		Pesticide L	Pesticide T	Pesticide L	Pesticide T	Influence
FREU	Freundlich exponent	4.5	107.2	9.7	357.8	+
KOM	Kom	4.6	81.8	7.7	190.1	-
DEG	Half life	3.8	34.6	7.8	112.7	+
ORG	organic matter content	3.0	13.8	4.1	20.8	-
BD	Bulk density	3.0	12.8	4.0	18.8	-
EGCV	Molar activation energy of degradation	4.1	10.0	5.8	16.2	+
LEDS	Lengths of dispersion in liquid phase	1.0	4.3	2.9	10.4	+
G6	Parameter n	2.8	1.3	8.0	4.0	+
G2	Saturated moisture content	1.8	1.5	5.4	1.8	-
COFR	Soil evaporation coefficient of Blak and Boesten or Boesten/Stroosnijder	0.162	0.914	0.309	1.8	-
CFTB	Crop factor	0.164	0.740	0.288	1.4	-
RDTB	maximum rooting depth	0.129	0.449	0.153	1.1	+/-
RDS	maximum rooting depth allowed by soil profile	0.052	0.356	0.074	0.893	+/-
SUWA	Coefficient of diffusion in water	0.129	0.165	0.307	0.749	+
RSIG	Minimum rainfall to reset models	0.026	0.396	0.074	0.828	+/-
G3	Saturated hydraulic conductivity	0.313	0.341	0.352	0.248	+
G1	Residual moisture content	0.515	0.165	0.184	0.093	-
G4	Alpha main drying curve	0.129	0.413	0.153	0.186	+/-
IF1	Extinction coefficient for diffuse visible light	0.057	0.248	0.153	0.233	+/-
IR1	Extinction coefficient for direct visible light	0.057	0.248	0.153	0.233	+/-
GCTB	Maximum leaf area index	0.052	0.165	0.153	0.233	+/-
PSI	silt content	0	0	0	0.581	+/-
CFLI	Coefficient describing the relationship between the conversion rate and the volume fraction of liquid	0.026	0.231	0.031	0.116	+
CFUP	Coefficient of uptake by plants	0.026	0.099	0.012	0.116	-
PSA	sand content	0	0.033	0	0.116	+/-
PCL	clay content	0	0.017	0	0.116	+/-
HI	initial pressure heads	0	0	0	0	
TEMI	initial soil temperatures	0	0	0	0	
RDD	Root density distribution	0	0	0	0	
THAI	Thickness of the stagnant air layer at soil surface	0	0	0	0	
SUAI	Coefficient of diffusion in air	0	0	0	0	
ENSL	Molar enthalpy of the dissolution process	0	0	0	0	
SAVP	Saturated vapour pressure	0	0	0	0	
ENVP	Molar enthalpy of the vaporisation process	0	0	0	0	

Table 41. Classification of PESTLA parameters according to their influence on pesticide losses (values presented are MAROV)

A positive influence means that an increase in the value of the parameter will result in an increase of recharge and vice versa

The shades of grey represent a classification of parameters into sensitivity classes as follows:

Extremely sensitive

Very sensitive

Moderately sensitive

Slightly sensitive

Insensitive

Results from the sensitivity analysis with regard to the prediction of percolation by PESTLA were only dependent on the soil type (*i.e.* the nature of the pesticide did not affect the ranking of parameters). A large number of input parameters affected the percolation predicted by PESTLA (12 parameters for the Wick soil, 9 parameters for the Hodnet soil), but their influence was rather small (MAROV values < 0.35). Influential variables included crop parameters (crop factor, extinction coefficients, maximum rooting depth, maximum leaf area index, maximum rooting depth allowed by the soil profile), parameters related to evapotranspiration (soil evaporation coefficient, minimum rainfall to reset models) and parameters related to the description of the water release characteristics (parameters for the Van Genuchten equation). Again, as noted for the other models, the main driver for the prediction of recharge will be the meteorological data which are provided to the model and parameters within the model will affect the predicted accumulated percolation to a small extent only. Although the coefficient for soil evaporation (know as CFBS in SWAP) was not included in the list of parameters to be varied, it is possible that this is an influential parameter. This parameter is helpful for correcting the conversion of potential evapotranspiration to actual evapotranspiration.

In contrast to the prediction of percolation by PESTLA, prediction of cumulative pesticide losses were greatly affected by changes in input parameters. The magnitude of the sensitivities was dependent on the different scenarios and was smallest for the scenario where the greatest losses were predicted (Pesticide L on Wick, maximum MAROV 5.9) and largest for the scenario where the smallest losses were predicted (Pesticide T on Hodnet (maximum MAROV ~360). In the fourth scenario, a modification of the Freundlich exponent from 0.9 to 0.99 resulted in an increase of pesticide losses from 0.043 g/ha to 0.864 g/ha.

Table 42 presents the 15 parameters which most influenced predictions for pesticide losses by PESTLA. There was a relative consistency in the ranking for the most sensitive parameters except for the third scenario involving Pesticide L in the Hodnet soil. The most sensitive parameters were generally those related to sorption (Freundlich coefficient and exponent) and degradation (half-life, molar activation energy of degradation). The organic matter content also had a significant influence since the description of sorption that was used in PESTLA for the four scenarios was that which made use of Kom and the organic matter content. In the third scenario involving Pesticide L in the Hodnet soil, the second most sensitive parameter was the dimensionless exponent “n” of the Van Genuchten equation which describes the water retention curve. Although the bulk density did not have any influence on the prediction of percolation volumes, it had a significant influence (MAROV>1) on the prediction of pesticide losses for all scenarios. The bulk density is used in the calculation of the repartition of the pesticide between the solid and liquid phases.

	ALW		ATW		ALH		ATH	
1	KOM	4.6	FREU	107.2	FREU	9.7	FREU	357.8
2	FREU	4.5	KOM	81.8	G6	8.0	KOM	190.1
3	EGCV	4.1	DEG	34.6	DEG	7.8	DEG	112.7
4	DEG	3.8	ORG	13.8	KOM	7.7	ORG	20.8
5	ORG	3.0	BD	12.8	EGCV	5.8	BD	18.8
6	BD	3.0	EGCV	10.0	G2	5.4	EGCV	16.2
7	G6	2.8	LEDS	4.3	ORG	4.1	LEDS	10.4
8	G2	1.8	G2	1.5	BD	4.0	G6	4.0
9	LEDS	1.0	G6	1.3	LEDS	2.9	COFR	1.8
10	G1	0.515	COFR	0.914	G3	0.352	G2	1.8
11	G3	0.313	CFTB	0.740	COFR	0.309	CFTB	1.4
12	CFTB	0.164	RDTB	0.449	SUWA	0.307	RDTB	1.1
13	COFR	0.162	G4	0.413	CFTB	0.288	RDS	0.893
14	RDTB	0.129	RSIG	0.396	G1	0.184	RSIG	0.828
15	SUWA	0.129	RDS	0.356	RDTB	0.153	SUWA	0.749

Table 42. The 15 most influential parameters on the prediction of pesticide losses by PESTLA for the four scenarios as determined by one-at-a-time sensitivity analysis (classification by MAROV values)

3.4.3 Results for the Monte Carlo sensitivity analysis

Descriptive statistics on the values for the PESTLA input parameters obtained via sampling into distribution functions are presented in Appendices 214 to 217. A total of 250 runs was carried out for each scenario using the randomly sampled values. Basic statistics on the percolation volumes and pesticide losses predicted by PESTLA are presented in Table 43. More detailed statistics are available in Appendices 218 to 228.

	Percolation (mm)				Pesticide losses (g/ha)			
	ALW	ATW	ALH	ATH	ALW	ATW	ALH	ATH
Minimum	2464	2408	2366	2326	5.5×10^{-3}	0	0	0
Mean	2657	2655	2637	2632	50	8.1	7.0	1.4
Median	2649	2648	2632	2632	33	0.5	2.8	0.04
Maximum	2970	2978	2968	2930	317	128	65	30
CV (%)	0.04	0.04	0.05	0.05	1.11	2.26	1.50	2.68

Table 43. Basic statistics on PESTLA predictions for the four scenarios

Regression techniques were used for non-transformed standardised data and transformed (ranked) standardised data. Coefficients of determination related to pesticide losses for the transformed data (r^2 0.92-0.95) were significantly larger than those for non-transformed data

(r^2 0.49-0.83) because of the inherent non-linearity in the prediction of pesticide losses by PESTLA. Classification of parameters according to their influence on the prediction of percolation and pesticide losses was therefore conducted using Standardised Rank Regression Coefficients only (Tables 44 and 45). The larger the absolute values of the regression coefficients (SRCC) the more influence the parameter has. An increase in a parameter with a positive SRCC will result in an increase in the model output and vice versa.

	ALW		ATW		ALH		ATH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
CFTB	-0.8496	1	-0.8908	1	-0.8454	1	-0.8762	1
IR1	-0.2046	2	-0.2188	2	-0.1320	5	-0.1848	4
COFR	-0.1646	4	-0.1988	4	-0.2429	3	-0.2357	3
RSIG	0.1451	5	0.1539	5	0.2692	2	0.2783	2
IF1	-0.1886	3	-0.2181	3	-0.1568	4	-0.1468	5
GCTB	-0.0462	9	-0.0336	11	-0.0604	6	-0.0613	6
G13	0.0938	6	0.0590	8	0.0394	7	0.0120	15
SAVP	-0.0237	17	-0.0206	15	0.0207	10	0.0474	8
RDS	-0.0846	7	-0.0564	9	-0.0169	15	0.0023	28
SUWA	0.0409	10	0.0362	10	-0.0108	20	-0.0076	19
G12	-0.0578	8	-0.0620	7	-0.0095	21	-0.0044	24
RDTB	-0.0358	12	-0.0690	6	-0.0118	19	0.0065	23
SUAI	0.0360	11	-0.0130	21	0.0159	16	0.0103	16
EGCV	0.0244	16	0.0284	14	0.0092	22	-0.0173	13
ENSL	0.0191	18	0.0314	12	-0.0071	25	0.0351	11
LEDS	0.0189	19	-0.0297	13	-0.0229	9	-0.0019	29
PSA	-0.0186	20	-0.0153	17	0.0196	11	-0.0041	25
TEMI	-0.0140	23	0.0055	26	0.0179	14	-0.0224	12
BD	0.0131	24	0.0138	18	-0.0152	18	-0.0066	21
CFUP	0.0101	27	-0.0010	32	0.0193	13	-0.0398	10
ORG	0.0349	13	0.0166	16	0.0076	24	0.0012	30
RDD	0.0113	26	-0.0130	20	0.0006	30	-0.0599	7
G16	0.0280	15	0.0041	30	-0.0194	12	-0.0026	27
ENVP	-0.0020	31	-0.0092	23	-0.0158	17	0.0173	14
G14	-0.0333	14	0.0099	22	-0.0009	29	0.0076	20
G11	0.0127	25	0.0132	19	0.0058	26	-0.0102	17
CFLI	-0.0084	28	0.0051	27	-0.0040	27	-0.0411	9
THAI	-0.0173	22	0.0068	24	-0.0086	23	0.0026	26
DEG	-0.0009	32	0.0046	28	0.0281	8	-0.0011	31
HI	0.0052	30	-0.0016	31	0.0035	28	0.0081	18
KOM	0.0183	21	0.0056	25	0.0005	31	0.0001	32
FREU	0.0073	29	-0.0041	29	0.0002	32	0.0065	22

Table 44. Classification of PESTLA input parameters according to their influence on results for percolation (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

	ALW		ATW		ALH		ATH	
	SRRC	Rank	SRRC	Rank	SRRC	Rank	SRRC	Rank
DEG	0.6633	1	0.3746	3	0.5904	1	0.4500	3
FREU	0.3333	3	0.5750	1	0.3528	4	0.6601	1
KOM	-0.5680	2	-0.4917	2	-0.4630	3	-0.4610	2
LEDS	0.2532	5	0.2041	4	0.4654	2	0.2139	4
EGCV	0.3110	4	0.1337	5	0.2495	5	0.1462	5
ORG	-0.0878	7	-0.0998	6	-0.0494	10	-0.0759	6
BD	-0.0636	9	-0.0901	7	-0.0484	11	-0.0481	9
G16	0.0294	12	0.0200	16	0.0897	7	0.0544	7
G12	-0.0883	6	0.0045	28	-0.0984	6	-0.0473	10
CFLI	-0.0259	16	0.0252	11	-0.0220	18	0.0404	12
G13	0.0676	8	0.0210	13	0.0268	16	0.0218	20
SUWA	0.0344	10	0.0153	20	0.0798	8	0.0209	21
IR1	0.0287	13	-0.0103	25	-0.0377	13	-0.0374	13
THAI	0.0269	15	0.0110	23	-0.0274	15	-0.0438	11
RSIG	0.0232	17	0.0171	17	0.0165	23	0.0534	8
G14	0.0134	19	-0.0632	8	-0.0200	21	0.0179	24
CFUP	-0.0283	14	0.0362	9	0.0161	24	0.0046	29
COFR	0.0118	21	-0.0306	10	0.0023	31	-0.0341	15
PSA	0.0093	22	-0.0153	21	-0.0448	12	-0.0202	22
RDTB	0.0070	24	-0.0155	19	0.0166	22	0.0262	16
SUAI	-0.0064	26	-0.0113	22	-0.0216	19	-0.0254	17
HI	-0.0015	29	0.0212	12	0.0134	26	0.0219	19
TEMI	0.0067	25	0.0168	18	-0.0222	17	-0.0059	28
CFTB	-0.0003	32	0.0206	15	-0.0088	28	-0.0356	14
GCTB	0.0004	31	0.0080	26	-0.0525	9	-0.0195	23
SAVP	-0.0147	18	0.0042	29	0.0347	14	0.0036	30
G11	-0.0129	20	0.0040	30	-0.0103	27	-0.0220	18
IF1	-0.0303	11	0.0002	32	0.0137	25	-0.0007	32
RDS	0.0055	27	-0.0210	14	0.0023	32	-0.0083	27
RDD	-0.0076	23	-0.0105	24	-0.0061	29	0.0103	26
ENSL	-0.0006	30	-0.0008	31	-0.0214	20	-0.0175	25
ENVP	-0.0053	28	-0.0068	27	-0.0049	30	-0.0021	31

Table 45. Classification of PESTLA input parameters according to their influence on results for pesticide losses (Monte Carlo sampling)
SRRC= Standardised Rank Regression Coefficients

Table 44 shows that only the five most influential parameters were consistent between the four different scenarios and contributed significantly to the sensitivity for the prediction of percolation volumes (|SRCC|>0.1). Predictions of percolation volumes were clearly dominated by the parameter CFTB, the crop factor at the development stage 1.5 and 2. There was a strong negative linear correlation between percolation volumes predicted by PESTLA and this particular parameter (r^2 0.73). The next four most influential parameters were the extinction coefficients for diffuse and direct visible light (IR1 and IF1, respectively), a soil evaporation coefficient (COFR) and a reset parameter (RSIG). The two former parameters

are needed to calculate the amount of light which reaches the canopy and the soil, which determines the rate of assimilation and soil evaporation. These two latter parameters are used in the calculation of the reduction of soil evaporation. Although the coefficient for soil evaporation (know as CFBS in SWAP) was not included in the list of parameters to be varied, it is likely that this is an influential parameter and that it has a significant influence on the prediction of percolation volumes.
Again, the Monte Carlo approach showed limitations in that all input parameters were assigned a sensitivity coefficient although most parameters were shown in the one-at-a-time sensitivity analysis to have no influence on the prediction of percolation volumes. Also, the use of a linear approach for describing the non-linear relationship between model input and output might have led to inaccuracies in the attribution of sensitivity indices.

A ranking of PESTLA parameters according to their influence on the prediction of pesticide losses is presented in Table 46. Ranking of the most influential parameters was somewhat affected by the scenario considered. A similar ranking for the five most influential parameters was obtained for the two scenarions involving Pesticide T. The five parameters which had the most influence on the prediction of pesticide losses by PESTLA were the Freundlich exponent (FREU) and distribution coefficient (KOM), the half-life (DEG), the molar activation energy of degradation (EGCV) and the length of dispersion in the liquid phase (LEDS). Although PESTLA was found to be sensitive to the first four of these parameters in the one-at-a-time sensitivity analysis, the length of dispersion was found to be somewhat less sensitive in the one-at-a-time sensitivity analysis.

	ALW		ATW		ALH		ATH	
1	DEG	0.663	FREU	0.575	DEG	0.590	FREU	0.660
2	KOM	-0.568	KOM	-0.492	LEDS	0.465	KOM	-0.461
3	FREU	0.333	DEG	0.375	KOM	-0.463	DEG	0.450
4	EGCV	0.311	LEDS	0.204	FREU	0.353	LEDS	0.214
5	LEDS	0.253	EGCV	0.134	EGCV	0.250	EGCV	0.146
6	G2	-0.088	ORG	-0.100	G2	-0.098	ORG	-0.076
7	ORG	-0.088	BD	-0.090	G6	0.090	G6	0.054
8	G3	0.068	G4	-0.063	SUWA	0.080	RSIG	0.053
9	BD	-0.064	CFUP	0.036	GCTB	-0.052	BD	-0.048
10	SUWA	0.034	COFR	-0.031	ORG	-0.049	G2	-0.047
11	IF1	-0.030	CFLI	0.025	BD	-0.048	THAI	-0.044
12	G6	0.029	HI	0.021	PSA	-0.045	CFLI	0.040
13	IR1	0.029	G3	0.021	IR1	-0.038	IR1	-0.037
14	CFUP	-0.028	RDS	-0.021	SAVP	0.035	CFTB	-0.036
15	THAI	0.027	CFTB	0.021	THAI	-0.027	COFR	-0.034

Table 46. The 15 most influential parameters on the prediction of pesticide losses by PESTLA for the four scenarios (Monte Carlo sampling).

4. SUMMARY OF FINDINGS

Sensitivity analyses of the four primary pesticide leaching models recommended for pesticide registration in Europe (MACRO, PELMO, PRZM and PESTLA) were carried out using two investigation methods (one-at-a-time and Monte Carlo sensitivity analysis) and four initial scenarios (2 pesticides, 2 soil types).

4.1 FINDINGS FOR INDIVIDUAL MODELS

4.1.1 MACRO 4.1

MACRO is the only model out of the four considered in this study which includes a description of preferential flow phenomena in soils.

A distinction in pesticide breakthrough was noted in the simulation of the initial scenarios. In contrast to the sandy loam soil where pesticide losses were predicted to occur over a few months in a year, pesticide breakthrough for the clay loam was characterised by large, but transient, losses. This led to larger losses in the clay loam compared to the less structured sandy loam, which is consistent with a larger influence of preferential flow phenomena on pesticide losses in the more structured soil.

Sensitivity of the MACRO model was found to be dependent on the scenario considered. Some parameters appeared to have a major influence for some scenarios and a smaller one in others. Also, the direction of the influence was found to depend on the scenario selected. Depending on the soil, the pesticide or the combination of the two, an increase in a specific input parameter resulted in either an increase or a decrease in pesticide losses.

Percolation volumes predicted by MACRO were much less affected by change in model input than pesticide losses. Sensitivity indices for percolation were less than unity which means that a given change in the input will result in a smaller change in the output. Percolation volumes were mostly affected by the parameter XMPOR which relates to the definition of the boundary between the two flow domains in MACRO. Crop parameters were also shown to have an influence on the prediction of percolation.

Predictions of total pesticide losses were much more affected by changes in input parameters. For the two scenarios involving the sandy loam, changes in pesticide losses were dominated by changes in sorption (Freundlich distribution coefficient and exponent) and degradation (degradation rates) parameters. These parameters have considerable uncertainty and this will contribute significantly to the uncertainty in modelling predictions. For the two scenarios involving the more structured clay loam, predictions for pesticide losses were also influenced by parameters related to the description of the hydrology of the soil. In one of the scenarios, these soil and hydrological parameters were more important in determining the loss of pesticides than sorption and transformation parameters.

4.1.2 PELMO 3.00

PELMO is a pesticide leaching model based on a “tipping bucket” hydrology and was developed from an early version of the PRZM model.

Simulations of the initial scenarios revealed that pesticide breakthrough profiles were not significantly affected by the soil type or pesticide considered. Only the time to breakthrough and number of years with leaching varied between scenarios. Total losses for a specific pesticide were predicted to be larger in the sandy loam than in the clay loam. Very small losses were simulated for the scenario describing the leaching of Pesticide T in the clay loam soil.

The magnitude of the influence of changes in model input on the prediction of recharge volumes was dependent on the soil type considered, but remained small. Simulated recharge volumes were affected by parameters related to the moisture content only (field capacity, wilting point and soil water content at the beginning of the simulation period). Crop parameters included in the sensitivity analysis had a very small effect on the prediction of recharge volumes.

In contrast to the prediction of recharge volumes, the prediction of pesticide losses by PELMO was extremely sensitive to changes in input parameters in most cases and the magnitude of sensitivity was dependent on the scenario considered. Extremely large indices of sensitivity were reported for one scenario, but this might be related to the very small losses predicted. Prediction of pesticide losses was mostly affected by degradation rates and sorption parameters (Freundlich coefficient and exponent). The field capacity also had a large influence on the prediction of pesticide losses for scenarios involving one of the two pesticides. Bulk density had a significant influence on the prediction of pesticide losses, although it did not affect the prediction of water volumes. This soil parameter is used in the calculation of pesticide losses by degradation and sorption processes.

4.1.3 PRZM 3.14b

PRZM is the pesticide leaching model recommended for submissions to the US regulatory authorities. It is based on a "tipping bucket" hydrology and has recently been modified to incorporate new subroutines such as a description of pesticide sorption by the Freundlich equation. In this study, the sensitivity of the model was investigated using a beta version of the model which was released in December 1999 with a shell to run the model for the FOCUS leaching scenarios.

PRZM simulations for the four initial scenarios showed that total losses for a specific pesticide were larger in the sandy loam than in the clay loam. Virtually no leaching of Pesticide T in the clay loam was predicted by the model. Pesticide breakthrough at the bottom of the soil cores was predicted to last longer for Pesticide T than for Pesticide L.

For all scenarios, recharge volumes predicted by PRZM were only affected to a small extent by changes in input parameters. The parameter with the largest influence on prediction of recharge was the "field capacity" which linked here both the field capacity for the soils and the soil moisture in the profile at the beginning of the simulation. Parameters which were found to influence the prediction of recharge were those related to the soil moisture status, to the computation of the actual evapotranspiration from the potential evapotranspiration and to the description of the crop cover.

In contrast to the prediction of recharge volumes, the prediction of total pesticide losses by PRZM was affected by a larger number of parameters and to a much greater extent. The largest sensitivities were reported for the scenario involving the clay loam, where pesticide losses were predicted to be smallest, but this is likely to be related to the small losses predicted. Although the most influential parameters were different for each scenario, the same parameters were found at the top of the list. These included the parameters related to pesticide sorption (Freundlich distribution coefficient and exponent) and degradation (degradation rates, QTEN) and, to a lesser extent, the parameters related to the description of the soil properties (field capacity, bulk density). These results agree with those found for the PELMO model as would be expected from the link in the development of the two models.

4.1.3 PESTLA 3.4

PESTLA is a pesticide leaching model which uses the hydrological component of the SWAP model. Description of water and solute transport is based on the Richards' equation and the convection-dispersion equation, respectively.

Simulations for the four initial scenarios showed that percolation volumes were predicted to be larger for the sandy loam than for the clay loam. The largest losses were predicted for Pesticide L in the sandy loam whilst the smallest losses were predicted for Pesticide T in the more structured clay loam. Leaching breakthrough for Pesticide L was shorter than that for Pesticide T.

Prediction of volumes of percolation by SWAP/PESTLA were found to be affected by a large number of parameters, but only to a small extent. Influential variables included crop parameters, parameters related to evapotranspiration and parameters related to the description of the water release characteristics. Although the coefficient for soil evaporation was not included in the list of parameters which were varied, it is anticipated that this parameter also has an influence on the prediction of recharge volumes.

In contrast to the prediction of percolation, prediction of total pesticide losses was greatly affected by changes in input parameters. The magnitude of the sensitivity was dependent on the scenario considered and was largest for the scenario where the smallest pesticide losses were predicted. There was a relative consistency in the list of the parameters which most influenced predictions for pesticide losses. The most influential parameters were those related to sorption and degradation (including both pesticide properties and soil organic matter content). Bulk density also had a significant influence on PESTLA/SWAP predictions for pesticide losses.

4.2 SUMMARY OF FINDINGS FOR ALL MODELS

The magnitude of sensitivity was found to differ between model output (*i.e.* percolation volumes or pesticide losses). For each model, the ranking of the input parameters by sensitivity of pesticide losses as well as the magnitude of the sensitivity itself were dependent on the scenario. The ranking of parameters was either dependent on the pesticide or soil considered or on both.

Model predictions for percolation were affected by a small number of input parameters and to only a small extent. Calculation of the potential evapotranspiration outside the model is likely to be the most important variable for the prediction of percolation volumes. In contrast, prediction of pesticide losses was found to be dependent on a large number of input parameters and was very much affected by variations in the model input. The magnitude of the sensitivities varied between the different models and the different scenarios. Overall model sensitivities for the different models were as follows: PELMO > PRZM > PESTLA > MACRO. The magnitude of the sensitivity appeared to be inversely related to the loss of pesticide by leaching (*i.e.* the smaller the losses, the larger the sensitivity). It therefore appears difficult to make a direct comparison of sensitivities between models since different levels of pesticide leaching were predicted by each. The largest absolute sensitivities reported may need to be considered as theoretical.

For almost all model-scenario combinations, parameters with the largest influence on pesticide predictions were those related to sorption (Freundlich coefficient and exponent) and degradation (either degradation rates or DT50, QTEN value). Most of these parameters have considerable uncertainty and they are likely to contribute greatly to the overall uncertainty in modelling predictions. Significant influence of some soil parameters (*e.g.* field capacity, bulk density) was also occasionally noted in some specific scenarios for all models. In one of the four scenarios for the prediction of pesticide losses by MACRO for a more structured clay loam, the influence of sorption and degradation parameters was surpassed by the influence of soil parameters specific to the definition of the boundary between micropores and macropores.

5. IMPLICATIONS FOR MODELLING ACTIVITIES AND SUBMISSION OF MODELLING STUDIES TO REGULATORY AUTHORITIES

5.1 USE OF THE DATA AND IMPLICATIONS FOR MODELLING ACTIVITIES

5.1.1 Robustness of results and applicability to other environmental scenarios

Results of a sensitivity analysis depend on the choices and specifications made throughout the analysis (*e.g.* parameters to include in the analysis, magnitude of variation of parameters, type of probability distribution functions (pdf's) for Monte Carlo sampling, parameterisation of pdf's). All choices can be rather subjective and arbitrary and this should be considered when applying the results obtained. Results from sensitivity analyses also depend on the initial scenario considered (the "base-case scenario"). This was confirmed by the investigations which were carried out within the scope of this project and this indicates the necessity of using multiple scenarios when studying the sensitivity of pesticide fate models. Although the four scenarios used in this study cover a range of conditions, they clearly do not encompass the full variability in environmental conditions to which pesticide leaching models will be applied. Detailed recommendations can be made on model sensitivity for percolation, but the complex interactions between soil hydrology, sorption and degradation makes it difficult to derive general rules for the loss of pesticides that would be applicable to a large range of soils or compounds. It is therefore recommended that information on sensitivity of models that has been derived here is used for scenarios which do not differ strongly from those considered in this study. For instances not covered (*e.g.* leaching of a volatile compound, loss of pesticides via drainflow), the information should be used as a rough guide only and it is recommended that quick sensitivity analyses are carried out for higher tier assessments.

Although a large number of model input parameters have been considered in the study, it was not possible to investigate all model parameters for practical reasons or because it was felt that there was no uncertainty on their values. It is known that some parameters not included in the investigations will significantly influence the prediction of percolation or pesticide losses. Examples include the application rate (it was not considered as an uncertain variable), the interception coefficient (no interception was considered, but this parameter is uncertain), the factors for the correction of degradation with depth (these were considered fixed, but they directly impact on degradation rates) and the compartment thickness (this can be used to indirectly introduce dispersion for some models). Although all these parameters are not present in the sensitivity tables produced within the scope of this project, care should be taken to ensure that adequate values are assigned to them.

5.1.2 One-at-a-time vs. Monte Carlo approach to evaluate model sensitivity

In this study, both one-at-a-time and Monte Carlo sensitivity analyses have been used to investigate the sensitivity of pesticide leaching models used for pesticide registration in Europe. Although this was not clear at the beginning of the investigations, it became apparent that the approach based on Monte Carlo approach has some disadvantages which may affect the influence which is attributed to individual parameters. The main flaw resides in the use of a linear regression model to derive sensitivity coefficients. The prediction of pesticide leaching is highly non-linear and this was apparent in the rather small distribution coefficients of the multiple linear regressions. A rank transformation successfully improved the goodness of fit indices, but it is not clear how much uncertainty is introduced by this transformation. Another problem lies in the attribution of a regression coefficient to all input parameters considered in the regression, even to those which do not affect model predictions as demonstrated in the one-at-a-time sensitivity analysis. Finally, there are some concerns regarding the reproducibility of the results obtained by Monte Carlo sensitivity analysis. It appears that the reproducibility is affected by both the seed numbers used for the generation of random values and by the number of sampled values.

One-at-a-time sensitivity analysis is intuitive and simple to conduct, but does not readily take into account the correlation between parameters (although this is feasible). It provides charts which give a quick visual assessment of sensitivity and which are easily understood by non-experts. Finally, the derivation of sensitivity indices from a one-at-a-time sensitivity analysis does not present issues related to the repeatability of the analysis.

Accordingly, it is concluded from this study that one-at-a-time sensitivity analysis should be the preferred option for investigating the sensitivity of pesticide leaching models. It is important to note that the inadequacy of the Monte Carlo approach only applies to the investigation of model sensitivity. Monte Carlo simulations remain valid within the scope of probabilistic risk assessment.

5.1.3 Calibration of pesticide leaching models

Calibration of models consists in varying selected input parameters and running the model until there is an acceptable fit between model predictions and experimental data. The selection of model parameters to be varied is usually left to the modeller and the calibration is rather subjective. It is recommended that the information on sensitivity provided in this report could be used to select those parameters which will be varied in situations similar to the scenarios considered here. In those instances where the situation differs significantly from those considered in this study, it is recommended that a rapid sensitivity analysis is carried out, either manually or automatically. Failure to understand which parameters most influence model predictions before engaging in a calibration task may result in an inadequate parameterisation of the model.

5.1.4 Rounding errors

Small modifications in model input can sometimes result in large variations in model predictions, especially when predicted pesticide losses are small. This implies that unwarranted rounding of values, especially for the most sensitive parameters (*e.g.* Kd and DT50 values, Freundlich exponent) should be avoided.

5.2 IMPLICATIONS FOR SUBMISSION OF MODELLING STUDIES TO REGULATORY AUTHORITIES

5.2.1 Confidence assigned to modelling studies and probabilistic approaches

Large sensitivities in the prediction of pesticide losses by leaching have been found for all four models used for the preparation of modelling submissions for pesticide registration in Europe even if the largest sensitivities were found for scenarios where little leaching was predicted. Given the large uncertainty associated with some of the most sensitive parameters, the outcome of any modelling study should be considered as uncertain.

Uncertainty is indirectly taken into account in the risk assessment for pesticides at lower tiers by the use of “uncertainty factors” (*e.g.* in the Toxicity Exposure Ratio approach). These factors attempt to compensate for the uncertainties in the risk assessment procedure (*e.g.* use of specific representative species to evaluate the ecotoxicology of a pesticide, uncertainty in the estimation of the exposure). The use of uncertainty factors at lower tiers is designed to provide a first-step screening of pesticides with regard to their effect on the environment and to identify those pesticides which need further risk characterisation. The approach is rapid and is considered adequate, although the magnitude of the factors is not based on any theoretical model and it is difficult to know the level of protection which is introduced. It is unlikely that the introduction of uncertainty considerations at this lower tier level would offer much benefit because of the relative complexity of taking uncertainty into account.

At higher tiers, mathematical modelling is heavily used to try to estimate the true potential of a compound to impact on the environment. More realistic assumptions are made and uncertainty factors may be correspondingly reduced. It is in these higher tier studies that there is a strong need for the inclusion of uncertainty considerations. Model output should be considered as uncertain and the influence of the uncertainty in the model input on the uncertainty of model output should be taken into account (*e.g.* by adopting a probabilistic approach).

5.2.2 Reporting needs

Selection of values for the most sensitive parameters is of great importance since small variations will significantly influence model predictions. Modelling studies should explicitly report the values for the most sensitive parameters and the way they were derived. Each choice should be carefully documented and justified. The origin of the value is important as large uncertainties can be found where non-specific pesticide or soil data are used (*e.g.* soil properties from databases or reference profiles). In those instances where no data are available, the influence of the uncertainty in the input parameters on model predictions could be taken into account at higher tiers by performing either a number of model runs for specific values of the most sensitive parameters or a full probabilistic risk assessment. Probabilistic risk assessment using a Monte Carlo approach should concentrate on the most sensitive and uncertain parameters.

5.2.3 Parameters and variables which require particular attention

Sensitivity analyses performed on pesticide leaching models revealed that, in most cases, the most influential parameters are those related to sorption and degradation. Parameters related to the soil moisture status were also found to have a significant influence on model predictions for pesticide losses in some instances.

The lack of major influence of model input parameters on the prediction of percolation/recharge volumes means that most care should be taken in the calculation of potential evapotranspiration outside the model. The balance between rainfall and evapotranspiration fed into the model will be the main driver of the prediction of recharge volumes.

The Freundlich exponent (referred to as “nf”, “n” or “1/n”) was found to have the largest influence on the prediction of pesticide losses for at least one scenario for three of the four models. However, assessment of leaching properties of a compound has traditionally largely focused on Koc/Kom and DT50 values. The importance of the Freundlich exponent should not be overlooked. This is a very influential and rather uncertain parameter and the selection for modelling of the mean value from a series of laboratory studies may not be scientifically justified.

A specific issue relates to the definition of the field capacity which was found to have a large influence on the prediction of pesticide losses for a number of models. The definition of field capacity with regard to its field determination is not universal and varies between countries. In Germany and the US, field capacity is defined as the water content at a pressure of -33 kPa, but different pressures are used in other countries (-5 kPa in the UK, -10 kPa in the Netherlands, -6 kPa in Canada). It is not clear which definition should be used for which models and a large uncertainty is therefore associated with this parameter. Again, an unambiguous reporting of the definition for field capacity which was used appears desirable in modelling submissions.

5.2.4 Development of standard scenarios

One of the ways to tackle large sensitivities and subsequent large uncertainties is to fix some parameters to default values. The use of standard scenarios where a large number of modelling parameters are fixed has been implemented by a number of countries (*e.g.* Denmark, Germany, the Netherlands). Scenarios for lower tier assessments have been recently developed by the FOCUS leaching group. It is important to note that results for these standard scenarios can still be largely influenced by small variations in the inputs which are not fixed (in particular pesticide parameters related to degradation and sorption) as leaching models are most sensitive to some of them. Recommendations on the selection of these parameters have been given by FOCUS (2000). The use of standard scenarios is only valid as a first-step assessment of the leaching character of a compound. It does not address sensitivity and uncertainty issues for higher tier modelling.

5.2.5 Sensitivity and uncertainty

This study investigated the sensitivity of the four models used for pesticide registration in Europe. Sensitivity and uncertainty are two modelling concepts which are closely linked and which are difficult to consider individually. Uncertainty considerations were included in the project through the definition of variation ranges for parameters (*i.e.* variation ranges were chosen to reflect the uncertainty in the parameter values) and this can be viewed as a simple first-step uncertainty analysis. The information derived on the sensitivity of pesticide leaching models in this study should be the starting point for further work to fully assess the uncertainty in modelling predictions and to develop procedures for performing probabilistic modelling (*i.e.* taking uncertainty into account).

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