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Comparing and evaluating pesticide leaching models: results for the Tor Mancina data set (Italy)

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Abstract

This paper describes the results of an evaluation of pesticide leaching modelling, using data collected on four lysimeters in Italy. The experimental data were collected during a 3 year period at Tor Mancina (Rome, Italy), on a clay-loam calcareous soil. Monitored variables are the soil water drainage, the bromide leaching and the metolachlor leaching. Two different irrigation schedules were considered in the experimental design. The models inadequately described the monitored breakthrough of water, bromide and pesticide. Poor modelling performance was firstly attributed to an inappropriate model structure, poorly representing the specific conditions of Mediterranean soils. In particular, the models did not allow to represent correctly the preferential flow that was observed during some of the flow events. Secondly, deficiencies were identified in the calibration procedures, and the application of a well defined modelling practice. The lack of such a good modelling practice induced user subjectivity in the estimation of the model parameters, which had an impact on the modelling results.

Keywords: Simulation models; Pesticides; Lysimeters; Percolation; Metolachlor; Bromide

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1. Introduction

Mediterranean countries, such as Italy, exhibits the highest water stress indicators of Europe (EU, 1998). The burden on the water resources is emphasised by irregular climatic conditions: long term dry periods are often irregularly interrupted by intensive storm events. The preservation of the long term quantity and quality of available freshwater resources, will therefore continue to play a crucial role in Mediterranean countries. In Italy, the pesticide pollution of the water resources varies in terms of the site specific soil and hydrological conditions. Leaching to groundwater is particularly important on the sandy soils, having shallow groundwater tables. Pesticide loading of the surface waters, as forced by erosion facilitated transport and runoff, will be more important in those areas which are characterised by steep slopes and heavy rainfall intensities.

Eighty seven percent of the drinking water in Italy is subtracted from groundwater. The need to safeguard the quality of the subsurface groundwater body against the potential adverse impacts of pesticides, is therefore extremely high. Therefore, a political commitment has been made to reduce the pesticide load to the fresh water body with 30–50%, mainly through a sound management of the pesticide use and the adoption of alternative crop protection methods (Imbroglini, 1991).

To improve the risk assessment of pesticide leaching to groundwater, both modelling and experimental studies should be carried out. Recently, the interest in lysimeter experiments has been increased (Hance and Führ, 1992). The leaching measured in lysimeters may be biased with respect to the leaching occurring in the field, since they do not consider the within field variability. In addition, the installation of range of lysimeters is very costly. On the contrary, lysimeter studies allow to monitor correctly the balance of different environmental variables, under controlled conditions. Lysimeter experiments can be repeated for a range of soil conditions, subjected to range of plausible boundary conditions. Further, it is generally accepted that the leaching observed in lysimeters may give a good indication on the vulnerability of a specific soil towards leaching. Finally, lysimeter data can be explored to evaluate the performance of point scale models predicting pesticide leaching.

In this paper, the performance is compared of five different pesticide leaching models, as used by six different model users, using data collected on four lysimeters, installed in Tor Mancina (Rome, Italy). The models are GLEAMS (Leonard et al., 1987), PELMO (Klein, 1995), SIMULAT (Diekkrüger, 1995), PRZM-2 (Mullins et al., 1993), and VARLEACH (Walker and Hollis, 1994). The evaluation was carried out in the framework of an intensive European test of pesticide leaching modelling. This exercise was initiated to support the adoption of pesticide leaching modelling technology in the framework of the registration, as suggested by the EU directives. Full details of the project, as well as the common modelling protocol are presented by Vanclooster et al. (2000). In this paper, details are only presented on the modelling studies carried out for the Tor Mancina data set.

2. Materials and methods

2.1. The data set

The details of the data set are described in detail in Francaviglia and Capri (2000). The experimental data were collected during a 3 year research period from May 1993 to June

1996, on a lysimeter installed in a clayey loamy calcareous fluvisol at Tor Mancina (Rome, Italy). The study was set-up to elucidate the potential risk of groundwater contamination from some herbicides commonly used in Mediterranean conditions (Capri et al., 1994, 1995; Francaviglia et al., 1996). Soil water drainage, soil bromide leaching and the concentration of metalochlor in the leachate was monitored. Metalochlor was applied in May 1993 and June 1995, as Dualin SP®. The applied amount was estimated to be 1.2 kg ha^{-1}. Bromide, in the form of NaBr and $CaBr_2$, was added at a rate of 100 kg ha^{-1} on May 1993, June 1994 and 1995. Details on the meteorological parameters, the soil conditions, and the crop and farm management, including the irrigation schedules, are given in Francaviglia and Capri (2000).

2.2. The models

For a detailed description of the models, the reader is referred to Vanclooster et al. (2000) and the papers referred therein. As well mechanistic leaching models (SIMULAT) and more empirical models (PRZM-2, VARLEACH, PELMO, GLEAMS) have been applied to the data set. The functional models, solves the soil water flow using a capacity type of approach. They are suggested to be used within the registration procedure (FOCUS, 1997). Preferential flow, which is considered to be important for many Mediterranean soils, is only considered within the SIMULAT model. This model is a fully mechanistic model solving the governing flow equation.

2.3. The evaluation procedure

Following the adopted modelling protocol (Vanclooster et al., 2000), model simulations were evaluated on the terms of the soil water balance, the soil solute balance, and the soil pesticide balance. Model users received the experimental data for 2 years (from May 1993 to May 1995) which enabled us to calibrate the model, and to evaluate the model user fitting's capacity. A 'blind' validation test was performed, using the experimental data of the third year. This allowed us to evaluate the prediction capacity of the model–user combination.

2.4. The model parametrisation

2.4.1. GLEAMS (GLF)

One single user used 2.10 version of the GLEAMS model. The Penman-Monteith equation was used to model evapotranspiration, since this equation is particularly suited for arid conditions (Leonard et al., 1987). However, for calculating evapotranspiration with the energy budget model of Penman-Monteith, both the mean wind velocity and vapour pressure deficit need to be known. These terms were estimated by the Tetens method as reported by Jensen et al. (1990).

Soil water parameters are given in Table 1. The values of the soil field capacity and wilting point were taken from the data set report. The saturated conductivity was reduced to the minimum default value of the model for the specific soil class. This allowed us to calibrate the initially overestimated soil water drainage.

Table 1
GLEAMS: hydrology-related input parameters and model switches

Parameter	Model user GLF
Fraction of plant available water (0–1)	0.20
Soil evaporation parameter (mm $day^{-0.5}$)	3.5
Rooting depth (cm)	100
Field capacity (cm cm^{-1})	0.42
Wilting point (cm cm^{-1})	0.32
Effective saturated conductivity (cm h^{-1})	0.13

The values of the Leaf Area Index (LAI) were taken from measurements collected at the surrounding field plots. It should be noted that the user manual does not report the default values of the LAI for broad bean and french bean. In addition, the default values for soybean, winter wheat and corn were low, compared to the common local data.

The sorption, degradation and plant uptake parameters for bromide and metalochlor were taken from the reference manual and the data base embedded within the model (Leonard et al., 1987). Values are reported in Table 2. No calibration was done on the sorption and degradation parameters, following the recommendations formulated by registration authorities.

2.4.2. PELMO

Two users (PEH AND PEK) performed five simulations with version 2.0 of the model. The adopted soil hydrological parameters and sorption and degradation parameters are reported in detail by Klein et al. (2000).

2.4.2.1. Model user PEK. The evapotranspiration rate was modelled with the Hamon equation, as reported by Carsel et al. (1984). This equation uses the daily temperature and light hour values to estimate the evapotranspiration rates.

The values of the soil field capacity and wilting point were taken from the data set report. The initial volumetric soil moisture content was set equal to 0.30 for all soil layers. For the bottom boundary condition, restricted drainage was considered. This was supported by the fact that a lysimeter does not exhibit free drainage conditions.

The default crop parameters of the model were used. The plant uptake factor for bromide was set at 0.1. The sorption and degradation data for bromide were ignored, and were taken from the data report for metalochlor.

Table 2
GLEAMS: input parameters for bromide and metolachlor (model user GLF)

Parameter	Bromide	Metolachlor
Water solubility (mg l^{-1})	>100 000	530
DT50 (days)	100 000	90
Koc	1	200
Plant uptake (%)	0.18	0

2.4.2.2. Model user PEH. Four individual simulations were carried out. For the first simulation, the pan evaporation data were used to estimate actual evapotranspiration rate. If no data were available, the Haude-equation was used (Haude, 1952). The Haude-equation only considers air temperature and vapour pressure deficit to force evapotranspiration. Crop specific parameters, parameters for the wind speed and radiation are lumped in an empirical correction factor. For the second simulation, the Haude-equation was used throughout the simulation. In a third simulation, parameters of the Haude-equation were calibrated. In a last simulation, the original Haude parameters were considered, while soil physical parameters were calibrated. In this case, soil bulk density was set equal to 1.0 g cm^{-3} while the field capacity was set to 0.62.

2.4.3. SIMULAT (SIA)

A calibrated and uncalibrated simulation run with 2.3 version of the model were presented. The Penman-Monteith model was used to estimate reference evapotranspiration. At the lower end of the lysimeter, free drainage was considered to occur. The soil physical parameters used in the model are given in Table 3. Water flow was simulated with the macropore module available in SIMULAT. With this approach, preferential flow through macropores will occur whenever the upper compartment is saturated. The saturated hydraulic conductivity was reduced from 6 to 1 cm per day for the first soil layer during the calibration phase of the model. This allowed macroporous flow to occur.

Maximum rooting depths of soybean, winter wheat, maize, fodder bean and french bean were set to 70, 100, 80, 70, and 50 cm, respectively.

For modelling the bromide fate, only convective–dispersive motion was considered. The dispersion length was set equal to 5 cm. The reference values of the soil water partitioning coefficient and half life, as given in the data set report, were used to model metalochlor sorption and degradation. The potential degradation rates will be reduced in terms of soil temperature and soil moisture content, following the relationships presented by Walker or Arrhenius (Richter et al., 1996). Volatilisation and plant uptake of bromide and metalochlor were ignored.

Table 3
Hydrology-related input parameters and macropore switches for SIMULAT

Hydraulic parameters	Model user SIA
Bulk density (g cm^{-3})	1.3 (0–10 cm), 1.4 (10–100 cm)
Thickness of compartments (cm)	5
Dispersion length (cm)	5
Initial water content (cm cm^{-1})	25
Van Genuchten/Mualem parameters	θ_s: 0.38 and θ_r: 0.18 cm cm^{-1}; α: 0.007 h Pa^{-1}; n: 1.3
Macropore model	
Macropore volume (cm cm^{-1})	0.05
Water flux in macropores (cm day^{-1})	200
Boundary condition	Free drainage, no lateral flow into soil matrix

2.4.4. PRZM-2 (PRT)

An empirical equation proposed by Mullins et al. (1993) was used to model evapotranspiration. In this equation the evapotranspiration rates can be limited by soil moisture availability. Free drainage was considered to occur at the lower boundary of the lysimeter. Soil layers with a thickness of 5 cm were considered. The values for the soil bulk density, the initial soil moisture content, the field capacity and wilting point, were set equal to 1.37 g cm^{-3} and, 0.186, 0.227, and 0.171, respectively. Default values for run-off were used, while erosion was not simulated. Standard values for the crop parameters were used. Rooting depth was set equal to 100 cm for all crops.

Bromide sorption and/or degradation was ignored. For the metolachlor fate, default parameters as given in the data set report, were used.

2.4.5. VARLEACH (VLE)

The Linacre equation (Linacre, 1977) was used to model actual evapotranspiration. Initial volumetric soil moisture was set equal to 0.31. Soil moisture at a pressure of 33.3 and 1500 kPa was set equal to 0.38 and 0.29, respectively. Bulk density was set equal to 1.238 g cm^{-3}. Crops were not considered in the model.

Since VARLEACH was not designed to model non-reactive solute transport, bromide fate was modelled by considering it as a soluble mobile pesticide component. Solubility was set to 100 000 mg l^{-1}. For metalochlor fate, the following parameters were used: solubility was set equal to 530 mg l^{-1}, while the soil-water partitioning coefficient was set to 2.05. Only one single application can be considered with the model.

3. Evaluation criteria

Both statistical and graphical model performance indicators were used. The modelling efficiency (EF) and coefficient of residual mass (CRM), as defined by Vanclooster et al. (2000) were used to qualify the simulated soil water drainage and bromide leaching. For metalochlor, these indices were not used since metalochlor leaching was not modelled by the capacity type models.

Since the differences between the two irrigation treatments and the four lysimeters were insignificant, they all were lumped in one single treatment in the calculation of one single statistic. For clustering the simulation results of the different models and model users in homogeneous groups, ANOVA techniques were applied and in particular multiple range analysis for the means of EF and CRM. Within this analysis, the least significant difference method and a 95% confidence level was adopted (Neter et al., 1985).

4. Results

4.1. Statistical indexes for water percolation and bromide leaching

The calculated model performance statistical indices and the clustering of these results in homogeneous groups, is presented in the Tables 4–7. The best fit for water percolation

Table 4
Mean EFs and multiple range analysis for cumulated water percolation

User	EF	Homogeneous groups			
PEH1	−7.308	X			
PRT	−3.098		X		
VLE	−2.104			X	
GLF	−0.055				X
PEH2	0.128				X
SIA1	0.448				X
SIA2	0.531				X
PEH3	0.542				X
PEH4	0.743				X
PEK	0.820				X

Table 5
Mean CRMs and multiple range analysis for cumulated water percolation

User	CRM	Homogeneous groups					
PEH1	−1.350	X					
PRT	−0.930		X				
VLE	−0.857		X				
PEH2	−0.327			X			
GLF	−0.310			X			
SIA1	−0.201			X	X		
PEH3	−0.182			X	X		
SIA2	−0.089				X	X	
PEK	0.023					X	X
PEH4	0.151						X

Table 6
Mean EFs and multiple range analysis for cumulated bromide leaching

User	EF	Homogeneous groups				
PEH2	−3.064	X				
PEH1	−2.751	X	X			
PEH3	−2.340		X			
SIA2	−0.532			X		
SIA1	−0.342			X	X	
PEH4	−0.286			X	X	
PEK	0.293				X	X
PRT	0.404					X
VLE[a]	0.537					X
GLF	0.725					X

[a] One application of bromide.

Table 7
Mean CRMs and multiple range analysis for cumulated bromide leaching.

User	CRM	Homogeneous groups			
PEH1	−0.808	X			
PEH2	−0.804	X			
PEH3	−0.692	X			
PEH4	−0.091		X		
PEK	−0.080		X		
SIA2	−0.047		X		
SIA1	0.015		X	X	
GLF	0.195			X	X
PRT	0.274				X
VLE[a]	0.333				X

[a] One application of bromide.

was obtained with the PELMO model, by model user PEK and with the fourth simulation of model user PEH. Mean EF were 0.82 and 0.74 respectively, while CRM are 0.023 and 0.151. The best fit for the simulated bromide leaching was obtained with the GLEAMS model: EF was 0.725 while CRM was 0.195. It should be noted that the well described water transport with the PELMO model does not correspond with an appropriate modelling of the bromide transport. It should further be noted that simulated plant water uptake of the bromide with the GLEAMS model was larger than the uptake simulated with the PELMO model which could explain this deviation.

The analysis of the EFs result in four homogeneous groups: simulation PEH1, PRT and VLE are significantly different among each other. The other simulations form one single group. The analysis of the CRMs show a slightly different result. While PEH1, PRT and VLE form the first two groups, the remaining simulations are clustered into four groups. Considering that the optimal value of CRM is zero, we can equally qualify the simulations PEK, PEH4 and SIA2.

Similar conclusions are drawn when analysing the statistics for the simulated bromide leaching. The multiple range analysis of EF result in a grouping of PEK, PRT, VLE and GLF in one single group. When CRMs are considered, SIA2, PEK and PEH4 are qualified to be equivalent.

4.2. *Comparative graphs*

4.2.1. *Metolachlor simulation*

Only SIMULAT simulated correctly the presence of metalochlor residues in the autumn of 1993 (Fig. 1). This could only be correctly represented when the saturated hydraulic conductivity of the first soil layer was calibrated, and preferential flow through macroporous was enabled. In late summer, little cracks were observed on the lysimeters, and therefore evidence for preferential flow exist (Francaviglia and Capri, 2000). Given the calibrated model, metalochlor breakthrough was simulated in the late summer of 1995, after a second application. However, such a breakthrough was not observed during this leaching event. The ‘blind model validation test’, therefore failed for the third year.

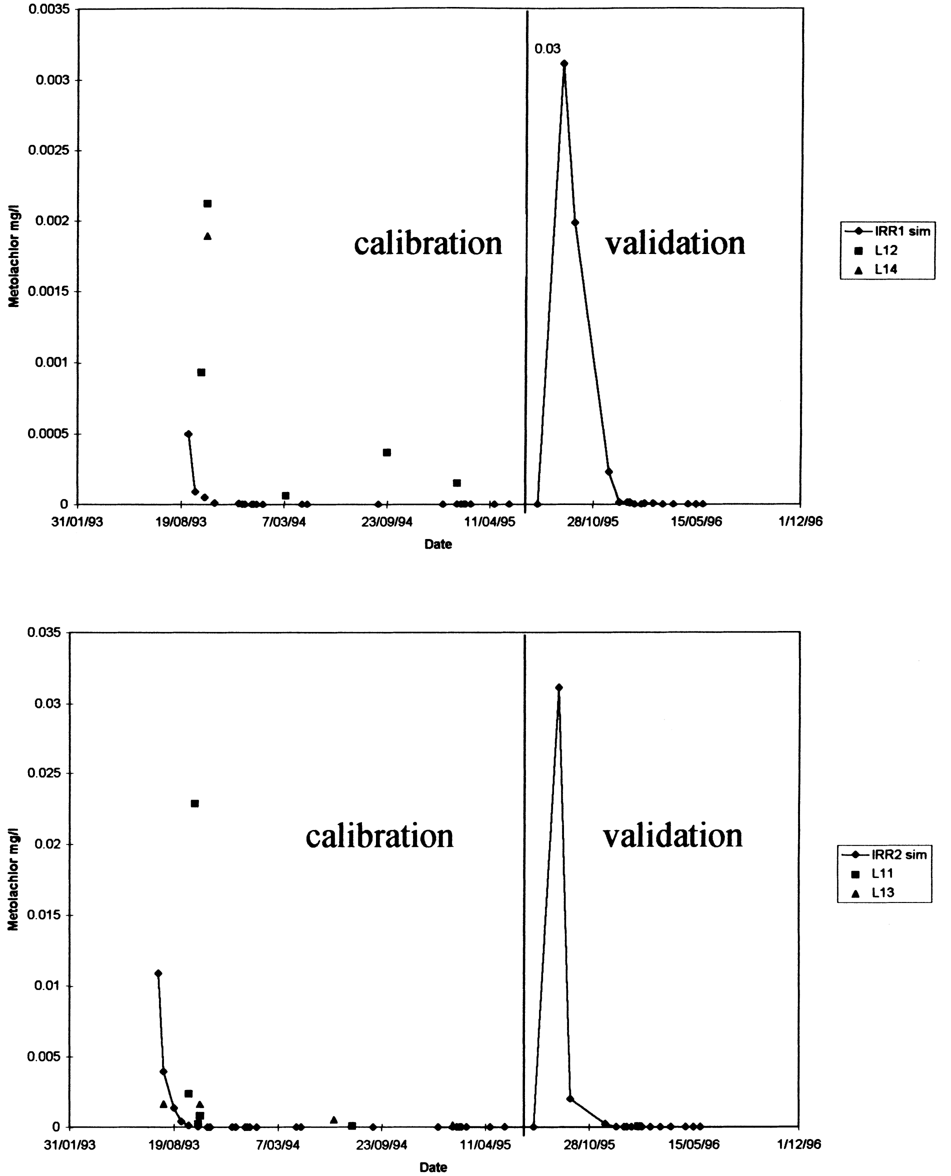
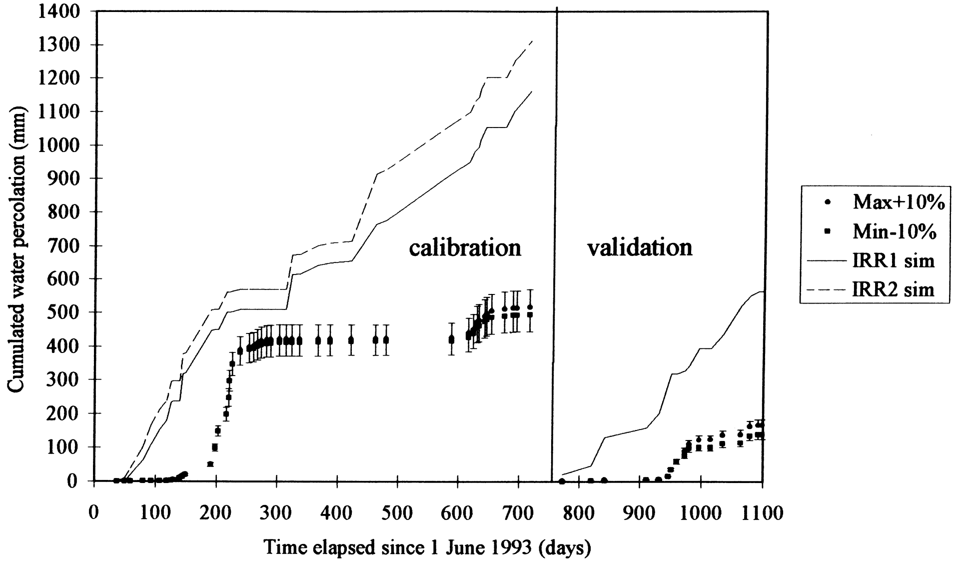


Fig. 1. SIMULAT, model user SIA. Calibrated results of simulations SIA2 for IRR1 (upper) and IRR2 (lower) irrigation treatments for metolachlor concentrations in mg l^{-1}.

4.2.2. Water percolation and bromide leaching

Details on the simulated percolation and bromide leaching for the two irrigation treatments are given in Figs. 2–6. In this paper, figures will be shown for PELMO, PRZM-2 and VARLEACH, to clarify the differences between different models and model



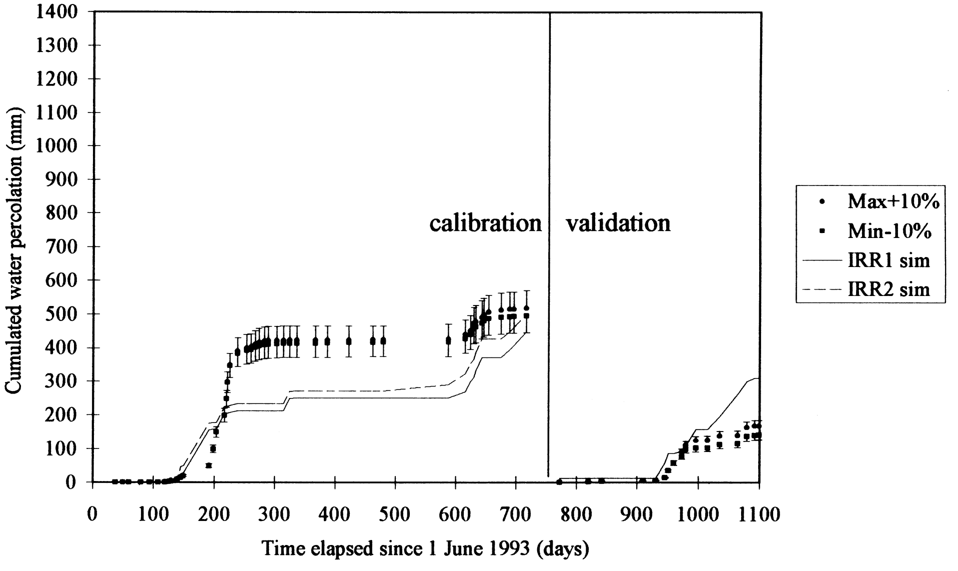


Fig. 2. PELMO, model user PEH. Results of simulations PEH1 (upper) and PEH4 (lower) for cumulated water percolation in mm.

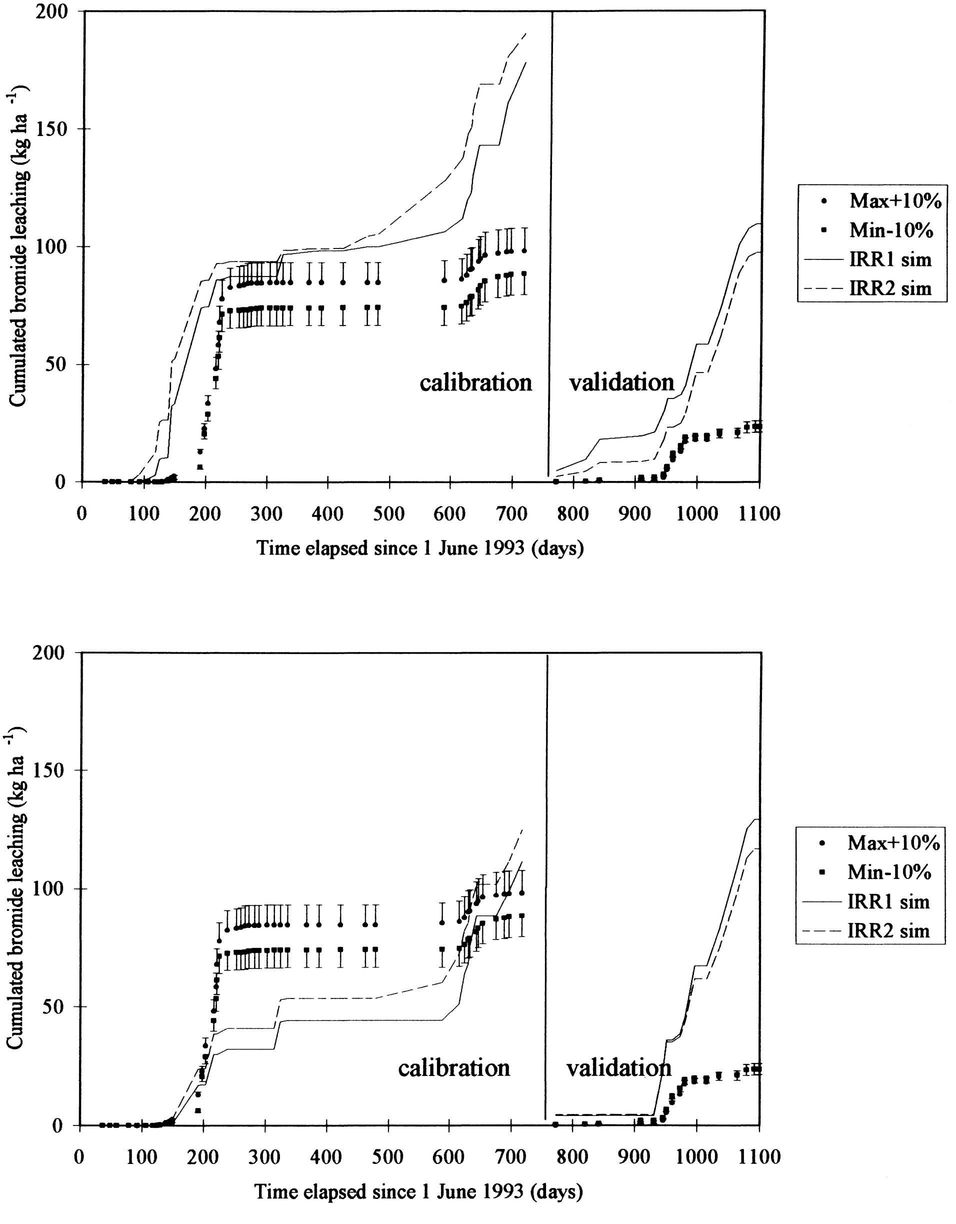


Fig. 3. PELMO, model user PEH. Results of simulations PEH1 (upper) and PEH4 (lower) for cumulated bromide leaching in kg ha^{-1}.

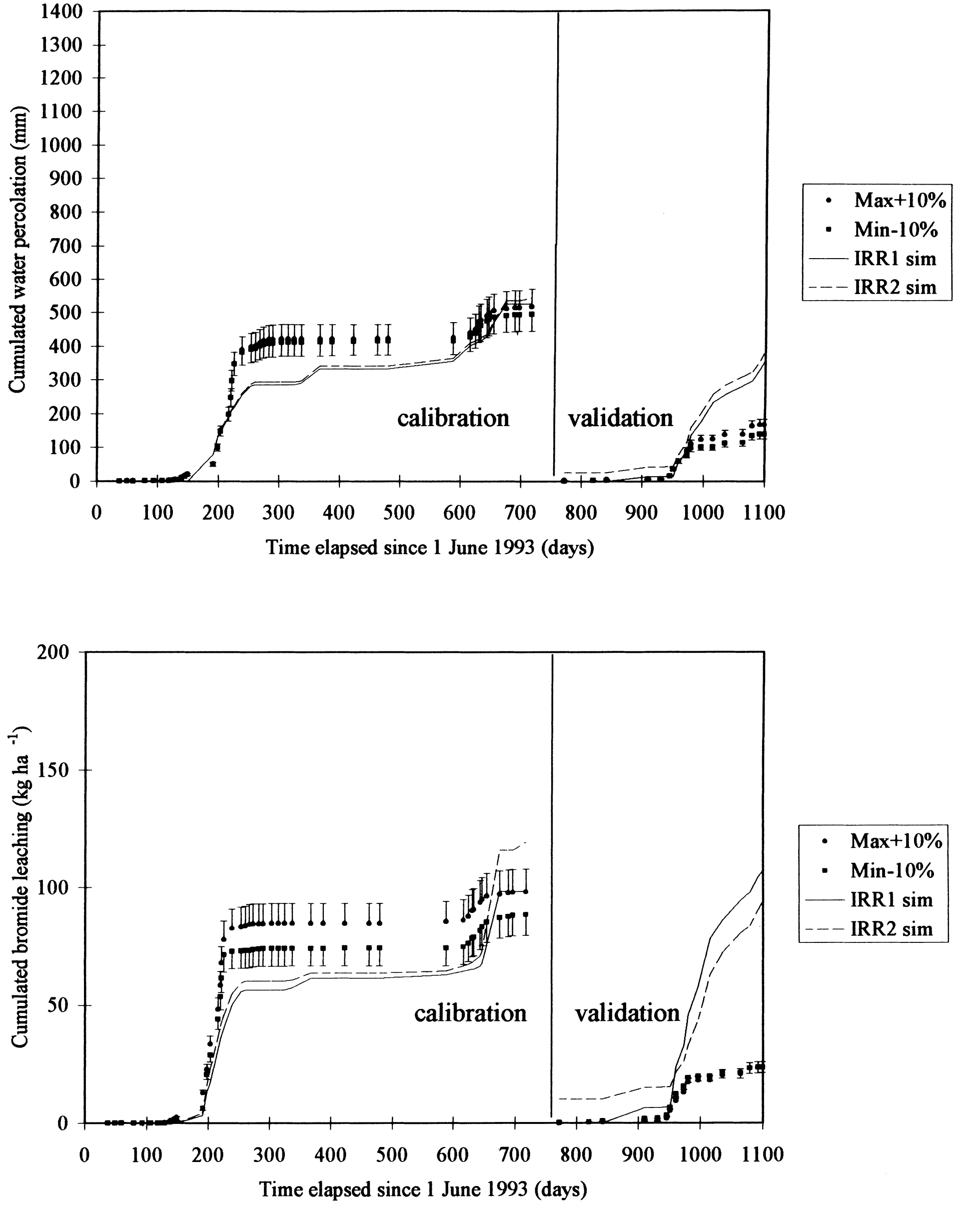


Fig. 4. PELMO, model user PEK. Calibrated simulations for cumulated water percolation in mm (upper) and bromide leaching in kg ha^{-1} (lower).

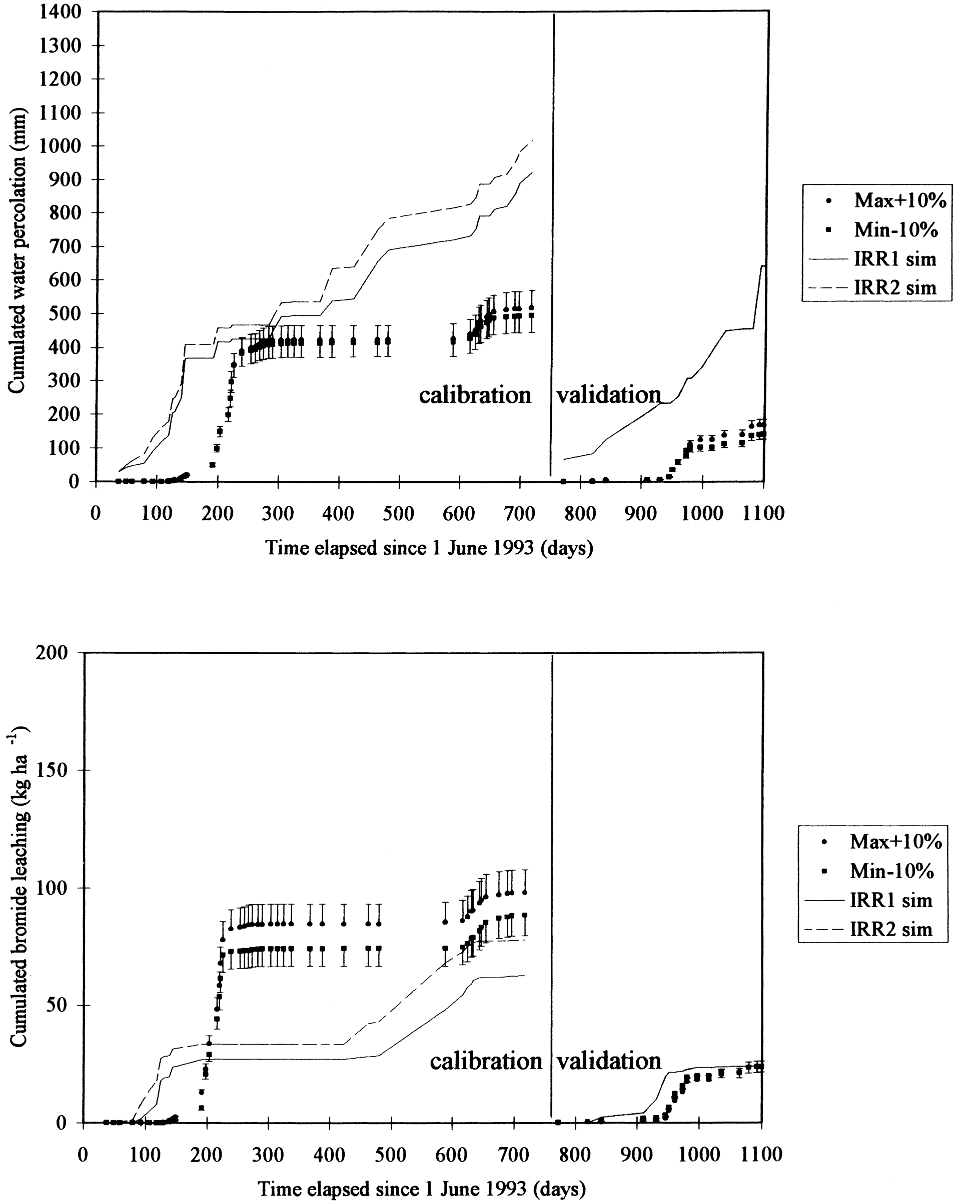


Fig. 5. PRZM-2, model user PRT. Calibrated simulations for cumulated water percolation in mm (upper) and bromide leaching in kg ha^{-1} (lower).

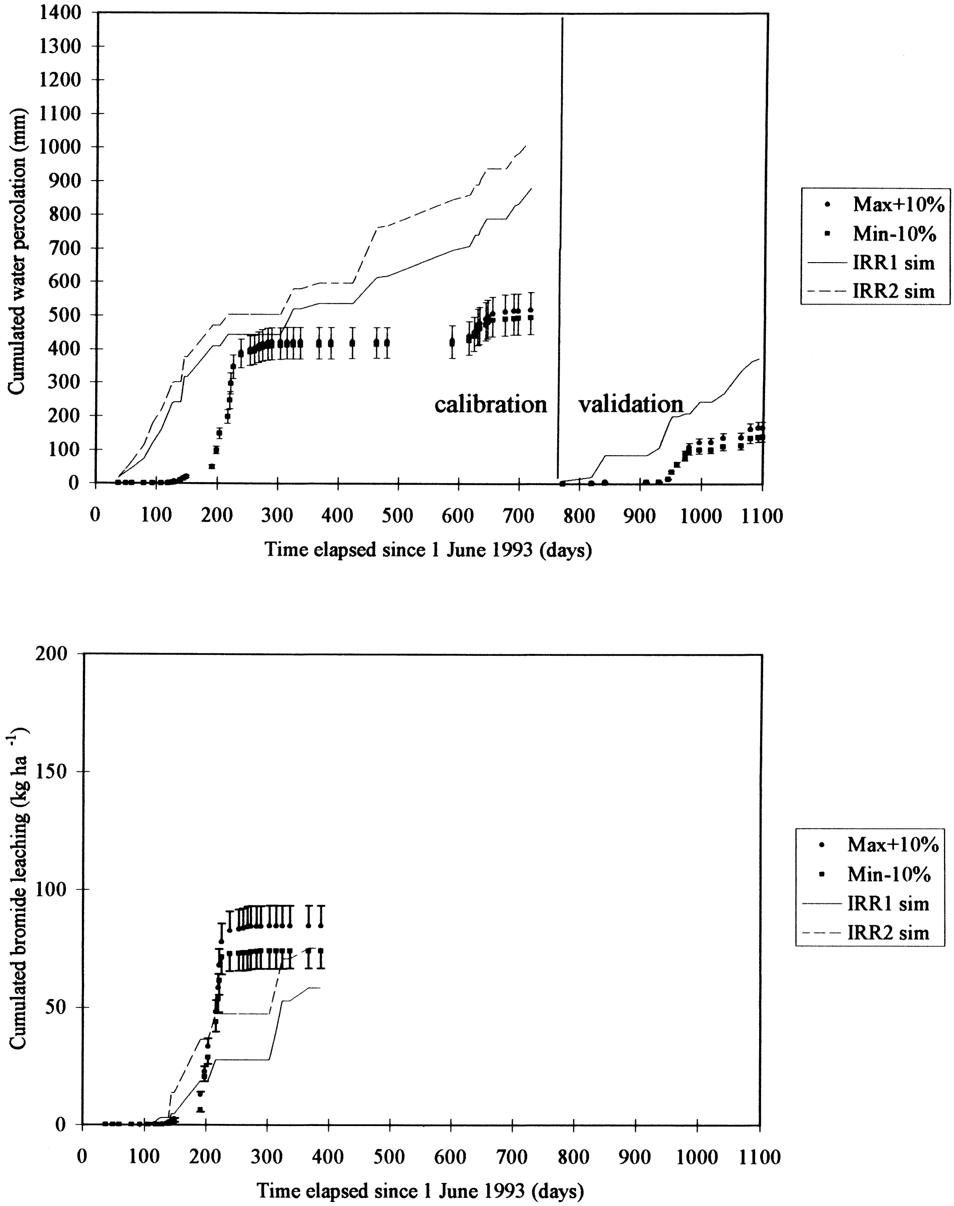


Fig. 6. VARLEACH, model user VLE. Calibrated simulations for cumulated water percolation in mm (upper) and bromide leaching in kg ha^{-1} (lower).

users. The maximum and minimum experimental values are given. The vertical bars represent the experimental error which is equal to 10%. The cumulative curves show the results for the calibration and the validation period. They restart from zero at the end of the calibration period to allow us to evaluate the absolute error during the validation test.

More details on PELMO, GLEAMS and SIMULAT simulations are given in the papers by Klein et al. (2000), Rekolainen et al. (2000), and Aden and Diekkrüger (2000).

Figs. 2 and 3 show the results obtained with PELMO by modeller PEH. Improvements of the modelling results were reported when calibrating the PELMO model, which confirms the analysis of the statistical indicators. This model user modified the given bulk density and field capacity to unrealistic values. This unrealistic values allowed the final values to be matched. However, the time course of the leaching was inappropriately represented. The validation of the third year also failed (Klein et al., 2000). Since no specific solute transport parameters were calibrated, similar conclusions can be drawn for the bromide breakthrough curve.

Results for PELMO by model user PEK are presented in Fig. 4. In contrary to PEH, PEK presented results which matched the time course of the soil water drainage curve appropriately. However, we judge again that the validation test failed. The better results for the PEK user during the calibration period can be ascribed to the choice of the model user to adopt the restricted drainage option and the setting of the minimum depth down to which soil water is extracted by the roots. The former mechanism causes the water to reside longer in the top layers where it is available for evapotranspiration, while the latter leads to more evaporation and therefore less leaching (Klein et al., 2000). The bromide leaching simulated by this model user was appropriately simulated during the first 2 years, but again the validation test failed.

The breakthrough curves for the GLEAMS model are reported by Rekolainen et al. (2000). They presented an acceptable simulation of the simulated water percolation. However, we judge that the validation failed on the third year.

Similar results for the SIMULAT model are presented by Aden and Diekkrüger (2000). We note however, that soil water flow parameters were calibrated, allowing to represent correctly the soil water breakthrough during the first 2 years. Yet, the validation on the third year failed. The lack of bromide parametrisation resulted in a complete lack of agreement all over the experiment.

Figs. 5 and 6 show the results of the PRZM-2 and VARLEACH model. Both models did not correctly simulate the percolation of water during the calibration and validation phase. On the contrary, bromide leaching simulated with PRZM-2 matched with the final measured values, and was considered acceptable for the validation. VARLEACH on the other hand, is conceived to consider only one single solute/pesticide application. Conclusions for the validation step could therefore not be drawn for this model.

5. Conclusions

From the results of the comparison of the models and model users, the following conclusions can be drawn:

- the movement of water in the soil is a key process in modelling pesticide leaching. However, a user dependent variability in the definition of the soil hydrologic parameters and boundary conditions has been observed. This is partly due to the subjectivity when identifying model parameters during the calibration phase of the model;

- some models, allowed to reconstruct appropriately the observed soil water and bromide breakthrough curves, but failed to predict these curves in a blind validation test;
- the PEK user of PELMO was able to reproduce reasonably well the water percolation through the lysimeter by controlling the evapotranspiration and drainage parameters;
- lysimeter experiments subjected to Mediterranean soil-climatic conditions are difficult to model with available pesticide leaching models. The considered models failed to describe the percolation of water when heavy rainfall events followed dry periods. They should therefore be judged inadequate for the description of water distribution in the soil profile;
- SIMULAT was the only model that reproduced correctly the occurrence of trace amounts of metalochlor, which were observed during the first 2 years in the lysimeter leachates. However, the model also predicted a metalochlor breakthrough during the third year, which has not been observed. The blind validation test therefore failed for this component of the model;
- preferential flow through macroporous soils should better be conceived in leaching models that are envisaged to be used in Mediterranean soil conditions.

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