Comparison of pesticide leaching models: results using the Weiherbach data set


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Abstract

The leaching of the herbicide isoproturon and the water tracer bromide in the profile of a silty loam soil at the Weiherbach Catchment area in Germany was simulated by eight different persons using the models MACRO, SIMULAT, LEACHP, WA VE, GLEAMS and PELMO (only bromide). Experimental results from different laboratory studies and from a field study were available to parameterise the models. Model results concerning water contents, tracer and pesticide profiles were provided for two different test periods in the field (winter and spring). The results for the behaviour of the herbicide and the tracer in the field study in spring were not known beforehand to the model users. Therefore this is considered to be a blind test.

After the model users had estimated the parameters and presented the modelling results a consensus parameter set was provided by the data set co-ordinator to reduce the subjective influence of individual users and to identify the effect of different model concepts.

The most striking points of the modelling exercise were the diversity of parameters estimated by different modellers from the same basic data set and the problems of simulating the field behaviour using laboratory derived pesticide parameters.

An overwhelming influence of the individual users on the model results was remarkable for the Weiherbach data set. It was not possible to estimate, from the laboratory data, alone a parameter combination suitable for describing the field behaviour of isoproturon satisfactorily. The use of
1. Introduction

This paper presents a comparison of models applied to data generated within the Weiherbach Project, Germany, in the context of the EU financed project COST Action 66 ‘Pesticides in the soil environment’.

Results of field experiments and lysimeters (lysimeters are not reported here) were available from the multidisciplinary research project ‘Weiherbach’ near Karlsruhe in the southwest of Germany. The objectives of the Weiherbach Project were the establishment of a high quality database to enable the development of numerical models describing all relevant water and solute fluxes, model parameterisation and model validation.

Over two experimental periods (winter 1993/1994 and spring 1995) water content, bromide concentration and the content of isoproturon were measured in the soil profile (0–95 cm) of a loess soil with macropores as well as in the leachate of lysimeters. Due to the fact that two tracer and pesticide applications were conducted the data were well qualified for calibration and validation of models.

The lack of multiple sets of good quality field studies specially designed for model validation with accompanying complete characterisation of soil hydraulic properties and pesticide-soil interactions was considered as the major obstacle for an objective model comparison. One of the data sets of the Weiherbach Project was initially ‘hidden’ from the modellers. Therefore it is possible to perform a blind test and an evaluation of the predictive capability of the different models. This ‘blind test’ is assumed to be one of the most effective model tests performed and published so far.

The parameter estimation process and the results of model applications are described. A comparison of the ability of the different models to simulate the hydrology of the site and the degradation and transport of isoproturon in the soil profile is presented.

2. Materials and methods

2.1. The Weiherbach data set

A description of the Weiherbach data set is given by Schierholz et al. (2000). Therefore only a short overview about the measurements used for parameter estimation and the experimental data which had to be predicted by the models is given in this report. The equipment for the field experiments was installed in winter 1993. Between December 1993 and June 1995 soil water content and soil temperature were continuously measured on a daily time scale at the field plot (referred to as Field Plot VIII). Isoproturon and bromide tracer were applied on a field in 1993. On nine sampling dates between 6/12/
1993 and 26/4/1994 the water contents, bromide contents and herbicide concentrations in soil were measured for 0–95 cm depth.

A second application of isoproturon was performed in 1995 on a separate field. Onto this field an additional irrigation of in total 260 mm was applied between 22/5/1995 and 19/6/1995. On 3 days per week a total maximum of 60 mm was added using a maximal irrigation rate of 4 mm h\(^{-1}\). To have a ‘blind test’ data set available, the results of the experiments in spring 1995 (11/5–23/6) were not made accessible to the model users before the provision of the modelling results, with the exception of IB (see Table 1) who was involved in the Weiherbach Project. Measurements of bromide and isoproturon in soil from seven sampling dates were available to the model users only after finishing the computer simulations for the ‘blind test’. Only the data of the soil water content in Field Plot VIII 1995 were accessible to the participants. So one period out of the two experimental periods was used for model calibration (1993/1994) and one for validation (1995).

Measurements of the water content and the bromide concentration in the experimental period 1993/1994 were given to calibrate the hydraulic parameters of the models. Parameters of the van Genuchten/Mualem retention and conductivity curves were provided, which had been identified from laboratory column measurements by inverse modelling.

Additionally laboratory experiments were available to identify sorption and degradation parameters of isoproturon in the Weiherbach soil. Various laboratory experiments were described and the model users had to choose between them and to estimate the model parameters by their own, e.g. isoproturon degradation experiments were conducted with soil sampled at three different times of the year. Due to this fact the predictive capability of the different models and the subjective influence of the individual users could contribute to the results. All users estimated parameters according to the protocol of the COST 66 workshop. A detailed description of the proposed validation procedure is given by Vanclooster et al. (2000a).

Each plot was covered with plants: in 1993/1994 and 1995 winter wheat and winter barley were grown, respectively. Different climatic parameters were measured — air temperature and air humidity, wind speed, potential evapotranspiration, global radiation, air pressure and rainfall. Minima, maxima and average values were available on a daily time scale. Precipitation was measured every 10 min.

2.2. Parameterisation procedure and models

Simulations of six different models MACRO, WAVE, LEACHP, GLEAMS 2.10, PELMO 2.01, and SIMULAT 2.3 are presented in this report. Two different versions 3.1 and 4.0 were used of one model (MACRO). Some models, e.g. MACRO, were used by different users. Table 1 gives an overview about the models and their users simulating the Weiherbach data set including the changing of parameters during the calibration process. The table lists the used half-life values and the sorption coefficient \(K_{OC}\) of the different computer runs. For the simulations with the uncalibrated hydraulic parameters the symbol ‘uncal’ is chosen meanwhile all other computer runs (‘cal 1’ and ‘cal 2’) were executed with calibrated hydraulic parameters. The expression ‘cal 2’ indicates that sorption and/or
Table 1
Models, model users and model parameters used for the simulation of the Weiherbach data set

<table>
<thead>
<tr>
<th>Model</th>
<th>Users and abbreviations</th>
<th>1993/1994</th>
<th>1995</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>uncal</td>
<td>cal 1</td>
</tr>
<tr>
<td>MACRO 4.0</td>
<td>C. Brown CB</td>
<td>( t = 23.5 ) days,</td>
<td>( t = 23.5 ) days,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( K_{OC} ) = 220</td>
<td>( K_{OC} ) = 220</td>
</tr>
<tr>
<td>MACRO 4.0</td>
<td>N. Jarvis NJ</td>
<td>( t = 16 ) days,</td>
<td>( t = 16 ) days,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( K_{OC} ) = 220</td>
<td>( K_{OC} ) = 220</td>
</tr>
<tr>
<td>MACRO 3.1</td>
<td>I. Bärlund IB</td>
<td>–</td>
<td>( t = 23 ) days,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( K_{OC} ) = 100</td>
<td>( K_{OC} ) = 100</td>
</tr>
<tr>
<td>LEACHP</td>
<td>M. Dust MD</td>
<td>( t = 14.7 ) days,</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( K_{OC} ) = 220</td>
<td>( K_{OC} ) = 220</td>
</tr>
<tr>
<td>WAVE</td>
<td>M. Dust MD</td>
<td>( t = 14.7 ) days,</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( K_{OC} ) = 220</td>
<td>( K_{OC} ) = 220</td>
</tr>
<tr>
<td>SIMULAT</td>
<td>K. Aden KA</td>
<td>( t = 35 ) days,</td>
<td>( t = 35 ) days,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( K_{OC} ) = 240</td>
<td>( K_{OC} ) = 440</td>
</tr>
<tr>
<td>GLEAMS</td>
<td>I. Bärlund, S. Rekolainen</td>
<td>IB, SR</td>
<td>–</td>
</tr>
<tr>
<td>PELMO</td>
<td>H. Schäfer HS</td>
<td>Only simulations of water and bromide</td>
<td>( K_{OC} ) = 91</td>
</tr>
<tr>
<td>PELMO</td>
<td>G. Görlitz GG</td>
<td>Only simulations of water and bromide</td>
<td>( K_{OC} ) = 91</td>
</tr>
</tbody>
</table>

\(^a K_{OC} =\) sorption coefficient (l kg\(^{-1}\)).
degradation parameters were changed by the model user. As an exception the calculations with the models WAVE and LEACHP must be mentioned, because all simulations were made with uncalibrated hydraulic parameters. Due to limited time of the model users the simulations with PELMO were only made for the soil moisture and bromide concentration of the first experimental period 1993/1994. A detailed description of the parameter estimation process and the changing of parameters during the calibration is described for every model below.

Three different simulation runs are reported in this paper — calculations with the uncalibrated and calibrated models for the experimental period 1993/1994 (soil moisture, bromide and isoproturon concentration), the results of the blind test for 1995 (soil moisture, bromide and isoproturon concentration) and the simulations using the hydraulic and pesticide parameters of the consensus data set for 1993/1994 and 1995 (isoproturon concentration).

The prescribed procedure implied a high degree of freedom for parameterisation by the individual model user. To reduce the huge variability of different parameters an additional simulation exercise was indicated. To eliminate the user subjectivity as much as possible, the wide range of pesticide parameters of the Weiherbach data set was reduced with a so called consensus parameter set that provided only one possible value for each pesticide parameter. This parameter set was provided by the data set co-ordinator after the simulation results of the blind test had been delivered. The parameters are given in Tables 2–4. The results of these computer runs, that should enable to evaluate the different models rather than the parameter estimation process, are referred to as ‘consensus’ results.

For the uncalibrated computer runs the hydraulic parameters as given in the data set or estimated from soil texture by a pedo-transfer function (PTF) were used without further calibration. Pesticide parameters were taken from laboratory experiments or from literature.

In the next step a calibration of the hydraulic parameters could be performed using the measurements of water content and bromide concentrations in soil from the experimental

Table 2
Input parameters (hydraulic parameters of consensus parameter set)a

<table>
<thead>
<tr>
<th>Hydraulic parameters</th>
<th>0–30 cm</th>
<th>&gt;30 cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_s ) (1 l l(^{-1}))</td>
<td>0.46</td>
<td>0.45</td>
</tr>
<tr>
<td>( \theta_r ) (1 l l(^{-1}))</td>
<td>0.03</td>
<td>0.08</td>
</tr>
<tr>
<td>( \alpha ) (l cm(^{-1}))</td>
<td>0.015</td>
<td>0.005</td>
</tr>
<tr>
<td>( n ) (–)</td>
<td>1.3</td>
<td>2.25</td>
</tr>
<tr>
<td>( K_s ) (cm h(^{-1}))</td>
<td>0.5</td>
<td>0.3</td>
</tr>
<tr>
<td>Volume fraction of water</td>
<td></td>
<td></td>
</tr>
<tr>
<td>At pF 1.8 (1 l l(^{-1}))</td>
<td>0.4</td>
<td>0.436</td>
</tr>
<tr>
<td>At pF 2.0 (1 l l(^{-1}))</td>
<td>0.372</td>
<td>0.413</td>
</tr>
<tr>
<td>At pF 4.2 (1 l l(^{-1}))</td>
<td>0.115</td>
<td>0.082</td>
</tr>
</tbody>
</table>

a Hydraulic parameters after van Genuchten/Mualem (van Genuchten, 1980): \( \theta_s \) is the saturated volumetric water content, \( \theta_r \) the residual volumetric water content, \( \alpha \) and \( n \) the empirical parameters, and \( K_s \) the saturated hydraulic conductivity. pF: volumetric water content relation for the parameterisation of cascade models.
period 1993/1994. The results of this computer run are referred to as calibration 1 in the text. Some modellers prepared an additional computer run with calibrated pesticide parameters (calibration 2), because they decided that a direct transfer of the results of the laboratory experiments to the field was difficult. They used additional information described in literature, e.g. sorption coefficient or half-life values of other field or laboratory experiments (outside the Weiherbach data set) to calibrate their models. For example MD calibrated parameters in WAVE and LEACHP which describe the influence of soil moisture on the degradation rate to obtain a better agreement between observed and calculated isoproturon concentration in soil.

A validation of the computer models was possible by predicting the measurements of 1995 (blind simulation). In this step no further calibration of the model was possible, because the model users did initially not have the measured results of the bromide and isoproturon concentration in soil. The hydraulic parameters estimated (and if necessary calibrated) from year 1993/1994 were used to simulate the conditions of 1995. As the simulation period 1995 is in spring/summer and the calibration term is in winter, some model users (CB in MACRO, IB in GLEAMS) corrected the rate coefficients for herbicide degradation because of different temperatures and microbial activity in soil.

### 2.2.1. MACRO

A detailed description of MACRO is given by Jarvis et al. (2000) and a short overview can be found in this issue. Three modellers used MACRO for their predictions — NJ and CB (MACRO 4.0) and IB (MACRO 3.1).

#### 2.2.1.1. MACRO 4.0 (NJ)

Hydraulic parameters were estimated from an experimental field plot ‘weather station site’ which had a soil texture similar to Field Plot VIII. Parameters which separate macropore and matrix flow like boundary hydraulic

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**Table 3**

Input parameters (sorption parameters of consensus parameter set)

<table>
<thead>
<tr>
<th>Sorption parameters&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Isoproturon $K_{OC}$ (l kg$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isoproturon $K_{OC}$ (l kg$^{-1}$)</td>
<td>119</td>
</tr>
</tbody>
</table>

<sup>a</sup>Linear sorption coefficient.

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**Table 4**

Input parameters (degradation parameters of consensus parameter set)

<table>
<thead>
<tr>
<th>Degradation parameters&lt;sup&gt;a&lt;/sup&gt;</th>
<th>$E_2$ (kJ mol$^{-1}$)</th>
<th>$\gamma$ (l K$^{-1}$)</th>
<th>Q10&lt;sup&gt;b&lt;/sup&gt; (--)</th>
<th>DT50 (10$^\circ$C) (days)</th>
<th>DT50 (20$^\circ$C) (days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isoproturon</td>
<td>58</td>
<td>0.13</td>
<td>3.6</td>
<td>65</td>
<td>16</td>
</tr>
</tbody>
</table>

<sup>a</sup>Factors are given to describe decreasing degradation rate with increasing soil depth (0–30 cm: 1; 30–50 cm: 0.9; 50–70 cm: 0.5; 70–90 cm: 0.3; >90 cm: no degradation occurs).

<sup>b</sup>Activation energy in Arrhenius law: $k = k_0 \exp(-E_2/RT)$.

<sup>c</sup>Parameter relating degradation rate to soil temperature, e.g. used by model PESTLA: $k = k_0 \exp(\gamma(T - T_0))$.

<sup>d</sup>Parameter used by some models: $k = k_0 \times Q10(T - T_0)/10$. 
conductivity and the boundary volume fraction of water and parameters related to the water uptake by crop roots were changed during the calibration procedure. Boundary conductivity was reduced from 3–5 to 1 mm h\(^{-1}\). No additional calibration was performed by NJ for simulation of Field Plot VIII. Default model parameter values for bromide were used throughout all simulations. The model user assumed a passive bromide uptake by plants.

For isoproturon a \(K_{OC}\) value of 220 l kg\(^{-1}\) was used in the uncalibrated model run. After calibration this value was reduced to 100 l kg\(^{-1}\) (cal 2). The average of measured degradation rate coefficients was used for isoproturon which is similar to a half-life of 16 days (at 20°C). In the further calibration the rate coefficient was increased to a value corresponding to a half-life of 8.1 days which is higher than the largest value measured in laboratory for the simulation period 1995. Parameter values for water and temperature response were derived from the measurements (\(\alpha = 0.118\) K\(^{-1}\) and \(B = 0.61\)).

The effect of temperature on degradation is described by an approach similar to the Arrhenius (formula 1) law where \(T\) and \(T_{ref}\) are the actual soil temperature and the reference temperature respectively (Jarvis, 1994)

\[
F_T = \exp(\alpha(T - T_{ref})).
\]

The influence of soil moisture is considered by following formula 2 (\(\theta\) stands for the actual water content and \(\theta_b\) for the boundary volume fraction of water)

\[
F_W = \left(\frac{\theta}{\theta_b}\right)^B.
\]

2.2.1.2. MACRO 4.0 (CB). Hydraulic parameters were determined by CB using PTF. Measurements of water content and bromide concentration in soil were used to calibrate the model.

For isoproturon a \(K_{OC}\) value of 220 l kg\(^{-1}\) was used in the uncalibrated model run. In the calibration procedure the sorption of isoproturon was changed to a \(K_{OC}\) of 90 l kg\(^{-1}\), according to literature (cal 2). Degradation parameters were obtained by CB fitting first order kinetics to the laboratory degradation data. For the top soil the half-life of isoproturon was 23.5 days at 20°C. The half-life was varied according to soil temperature and moisture content using MACRO default values for the response functions (\(\alpha = 0.08\) K\(^{-1}\) and \(B = 0.7\)). For simulation run ‘cal 2’ the influence of temperature and soil moisture on the degradation rate were switched off.

For the blind simulation of the experiment in 1995 CB reduced the topsoil half-life of isoproturon to 50% of winter value (i.e. 11.75 days) using expert judgement.

The degradation rate in the model was assumed to decrease down the profile according to the organic carbon content in soil. The user assumed that there was no uptake of either bromide or isoproturon by the crop.

2.2.1.3. MACRO 3.1 (IB). IB used reported measurements from the Weiherbach Project for estimating hydraulic parameters. Brooks & Corey parameters were derived from given van Genuchten/Mualem parameters. In comparison to other MACRO users a high \(\Psi_b\)-value (boundary soil water pressure head) was used. A higher saturated
conductivity (5 cm h\(^{-1}\)) than measured (0.5 cm h\(^{-1}\)) was chosen which should represent the soil texture in the field better than measurements of conductivity in small soil columns.

For isoproturon a linear sorption coefficient (\(K_d\)-value) of 1.05 l kg\(^{-1}\) was estimated for the uppermost 25 cm and a \(K_d\)-value of 0.45 kg l\(^{-1}\) was considered for deeper layers, derived from a \(K_{OC}\) of 91 l kg\(^{-1}\). Degradation was described by first order kinetics assuming a half-life of 23 days for the top soil in the winter period 1993/1994 (cal 1) and a half-life of 16 days for the experiment in spring 1995 (cal 2). In contrast to all other model users the results of the 1995 experiment were known to IB. Influences of temperature and humidity on the degradation rate were considered by using default values in MACRO (\(a = 0.08\) K\(^{-1}\) and \(B = 0.7\)). The degradation rate in the soil profile was assumed to decrease according to the organic carbon content of the different layers.

In the model a plant uptake coefficient of 0.1 was chosen for bromide and isoproturon.

2.2.2. WAVE (MD)

Vanclooster et al. (2000b) give a detailed description of WAVE. For the uncalibrated and the calibrated model run the van Genuchten/Mualem hydraulic parameters of the Weiherbach data set were used directly as reported. For isoproturon a \(K_d\)-value of 2 l kg\(^{-1}\) was chosen for the uppermost 25 cm and 1.69 l kg\(^{-1}\) for deeper soil layers (\(K_{OC} = 220\) l kg\(^{-1}\)). For the 0–30 cm a half-life of 14.7 days and for the 30–95 cm layer a half-life of 139 (at 25°C) days were estimated from the laboratory incubation experiments. Response terms were used to reduce the potential degradation rate constants according to the actual soil temperature and soil moisture. A calibration of the pesticide parameters was made by correcting the Parameter \(b\), which describes the relation between degradation rate and soil moisture. An initial value of 0.715 estimated from laboratory experiments was changed to 0.2. Volatilisation and plant uptake were not considered for bromide or isoproturon.

2.2.3. LEACHP (MD)

A description of LEACHP is given by Dust et al. (2000). Hydraulic parameters of van Genuchten/Mualem were directly taken from the Weiherbach report and not changed during the calibration process. Linear sorption parameters were also taken from the laboratory experiments — a \(K_d\)-value of 2 l kg\(^{-1}\) for the uppermost 0–30 cm layer and 1.69 l kg\(^{-1}\) for depths greater than 30 cm (\(K_{OC} = 220\) l kg\(^{-1}\)). Degradation parameters were changed for isoproturon during calibration — the half-life of 14.7 days for top soil was reduced to 7.4 days and for deeper soil layers the half-life values decreased from 138.6 to 69.3 days based on a reference temperature of 20°C. Additionally soil moisture correction factors were changed. Volatilisation and plant uptake were not considered for bromide or isoproturon.

2.2.4. GLEAMS 2.1 (SR & IB)

A description of the GLEAMS model is given by Leonard et al. (1987) and Rekolainen et al. (2000). For the uncalibrated model run the field capacity and the wilting point were used as measured in the Weiherbach soil. During calibration the field capacity
was reduced according to the specific soil texture using PTF in the GLEAMS manual (cal 1).

For all simulations a $K_{OC}$-value of 911 kg$^{-1}$ was used, except for the consensus simulation where the $K_{OC}$ of 1191 kg$^{-1}$ was considered. Due to different environmental conditions between winter and summer different half-life values were used. For the winter and the summer period half-lives of 23 days and of 8 days were assumed, respectively. For depths greater than 25 cm the degradation rate was decreased. For the consensus data set the suggested half-lives were used. A plant uptake coefficient of 0.1 was chosen for isoproturon and bromide. No volatilisation was considered.

2.2.5. SIMULAT 2.3 (KA)

A description of SIMULAT is given by Diekkrüger et al. (1995) and by Aden and Diekkrüger (2000) (this volume). For the uncalibrated computer runs the hydraulic parameters of van Genuchten/Mualem given in the Weiherbach data set were used. For calibration only the measurements of soil moisture and bromide transport of Field Plot VIII 1993/1994 were considered. During the calibration process the soil was subdivided into six soil layers instead of two and the saturated conductivity was increased from 0.5 to 3 cm h$^{-1}$ for the 0–30 cm layer and from 0.3 to 4 cm h$^{-1}$ for deeper layers. Additionally an approach for mobile–immobile water content was used. An immobile volume fraction of water of 0.07 cm$^3$ cm$^{-3}$ was assumed. A macropore model option was not chosen because the transport of bromide 1993/1994 in soil could be predicted correctly using matrix flow and the mobile–immobile approach only.

For all simulations (except the consensus parameter set where a first order kinetics was used to simulate degradation as suggested) microbial degradation was assumed for isoproturon. In contrast to all other models the dynamics of microbial activity (that controls the degradation) was simulated separately, using informations from the lab study (see Diekkrüger et al., 1995). Laboratory data show an evident lag phase and different authors reported a microbial degradation for this pesticide. Model parameters which describe the dynamics of microbial activity in soil were estimated from the laboratory experiments. A half-life of 35 days (at 20°C) and a linear sorption coefficient of 4 ($K_{OC} = 4401$ kg$^{-1}$) was used. The influence of soil moisture and temperature on the degradation rate is considered in the model as estimated from the Weiherbach data set. Plant uptake or volatilisation was not considered in SIMULAT.

2.2.6. PELMO 2.01

A description of PELMO is given by Klein et al. (2000). Two persons used PELMO: HS and GG. Only simulation results for the water content and the bromide concentration of Field Plot VIII 1993/1994 can be presented in this report.

2.2.6.1. PELMO (HS). Hydraulic parameters were estimated with different methods. For bromide a $K_{OC}$-value of zero and a half-life of 3000 days was assumed. Table 5 gives an overview about hydraulic model parameters that were used.

2.2.6.2. PELMO (GG). Hydraulic model parameters were estimated from the Weiherbach data set without further calibration.
2.3. Statistical coefficients for comparison

A visual comparison of results is often subjective and goodness-of-fit criteria are required. For example it must be defined if the absolute pesticide content in soil should be predicted or if the transport is much more important. In the latter case the maximum peak depth can be used for evaluation of the model results.

In Figs. 4, 6 and 8 some examples of model calculations in comparison with the measurements are shown to give an impression of simulation results of the experimental period 1995 which is provided for model validation. In addition, numerical comparisons of modelling results with observed values are provided. But goodness-of-fit indexes also show up difficulties when used for this kind of comparisons. Therefore more than one statistical index is given in this report. All sampling days are summarised. The formulas of ‘model efficiency’ (ME) and ‘coefficient of determination’ (CD) are given by Vanclooster et al. (2000a,b).

Values between $-\infty$ and 1 (=optimal value) can be calculated for the index ME, which gives an impression of the overall fit of the model. The predicted distribution of pesticides in the soil profile in comparison to measurements can be evaluated with the index CD. The optimum value for CD is 1. If model predictions deviate only with respect to the position in profile but not in absolute value an index of 1 also can be reached.

Model efficiencies were calculated for each sampling date and results were summarised in Box and Whisker Plots (=‘box plots’). The cycles indicate minimal and maximal ME. 10 and 90 percentiles are shown by lines and the box defines the 25 and the 75 percentile. The horizontal line marks the median value (50 percentile).

<table>
<thead>
<tr>
<th>Computer run</th>
<th>Calculation of potential evapotranspiration</th>
<th>Water retention parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Volumetric water content at field capacity (1 $\text{l}^{-1}$)</td>
</tr>
<tr>
<td>PELMO 1</td>
<td>After Hamon$^a$</td>
<td>0.400$^b$ (0–25 cm)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.436$^b$ (0–95 cm)</td>
</tr>
<tr>
<td>PELMO 2</td>
<td>After Haude$^c$</td>
<td>0.414$^d$ (0–95 cm)</td>
</tr>
<tr>
<td>PELMO 3</td>
<td>After Haude</td>
<td>0.319$^e$ (0–25 cm)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.311$^e$ (25–95 cm)</td>
</tr>
<tr>
<td>PELMO 4</td>
<td>After Hamon</td>
<td>0.319$^e$ (0–25 cm)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.311$^e$ (25–95 cm)</td>
</tr>
<tr>
<td>PELMO 5</td>
<td>After Hamon</td>
<td>0.414$^d$ (0–95 cm)</td>
</tr>
</tbody>
</table>

$^a$ Potential evapotranspiration is calculated using the air temperature (see Klein, 1995).
$^b$ Measurements, reported in Weiherbach data set.
$^c$ Potential evapotranspiration is calculated using the air temperature, air humidity and plant parameters (see Klein, 1995).
$^d$ Estimated with FhG-correlation from soil texture (PTF, see Klein, 1995).
$^e$ Estimated with PRZM-correlation from soil texture (PTF, see Klein, 1995 and Mullins et al., 1993).
3. Results

Not all the participating model users carried out all of the suggested computer runs. The highest number of simulations is available for 1993/1994 winter period, concerning water content and bromide concentration in soil. For GLEAMS, MACRO (IB), WAVE and LEACHP only simulation results with calibrated hydraulic parameters or modified degradation parameters were reported. The model PELMO was used only to calculate water content and bromide concentration in soil in the experimental period 1993/1994.

For the three models SIMULAT, MACRO (IB and CB) and GLEAMS the simulation results for the ‘consensus parameter set’ can also be presented.

As one example of the goodness-of-fit parameters the ‘Model efficiencies’ were calculated from the simulation results of bromide concentration and soil moisture. For isoproturon additionally the index ‘CD’, is reported.


The best fit for soil moisture was obtained with the calibrated model SIMULAT (cal 1) and MACRO (CB, cal 1). Mean ME are 0.113 and 0.088, as listed in Fig. 1. The box plots of all sampling dates shown in Fig. 1 also indicate good agreement between calculations and measurements for these two models. Following models show similar ME between $-0.058$ (LEACHP) and $-0.898$ (PELMO run 4) — LEACHP, SIMULAT (uncal), GLEAMS, MACRO (IB), WAVE, PELMO (run 3 and 4). MACRO (NJ, uncal, cal), uncalibrated MACRO (CB) and the other PELMO simulations could not predict the water dynamic in soil in a satisfying way. Mean ME are between $-4.440$ and $-8.661$.

3.1.2. Bromide concentration in soil 1993/1994

Model efficiencies calculated from bromide predictions are provided in Fig. 2. Additionally, the range of ME for each sampling date 1993/1994 is summarised in box plot graphs.

The results of the uncalibrated and the calibrated simulations are printed in the same graph. The influence of the calibration procedure on the quality of the predictions is obvious, if you compare the ME box plots of MACRO CB (MACBu and MACBc), MACRO NJ (MANJu and MANJc) or SIMULAT (SIKAu and SIKAc) in Fig. 2.

Fig. 2 shows model efficiencies between 0.455 and 0.571 for the uncalibrated model SIMULAT and MACRO (NJ, CB). After calibration all three model users reached model efficiencies greater than 0.7. MACRO (IB), GLEAMS and PELMO (run 3 and 4) also provided similar good predictions of bromide transport in soil. Simulations with the calibrated model MACRO (CB), gave the best results.

From the simulation results of LEACHP and WAVE an ME of 0.641 and of 0.57 was calculated. It has to be mentioned that the models were not further calibrated. The model parameters were directly derived from the Weiherbach data set. In comparison to other uncalibrated models like PELMO (except PELMO run 3 and 4) and SIMULAT these results are very good. For WAVE and LEACHP the range of ME calculated for each sampling day is quite small.
Fig. 1. Box plots of model efficiencies for calculating soil moisture content 1993/1994.
Fig. 2. Box plots of model efficiencies for calculating bromide concentration in soil 1993/1994.
PELMO gave the worst description of bromide transport in soil, with the exceptions of PELMO run 3 and 4 (HS). It has to be mentioned that the PELMO users could spend only a limited time in their modelling efforts for Weiherbach and made no calibration. They only used different methods to obtain hydraulic parameters from the soil texture.

3.1.3. Isoproturon concentration in soil 1993/1994

The main aim of the workshop was the comparison of models according to their ability to predict pesticide behaviour in soil. Table 6 lists two statistical coefficients (ME and CD) to compare the simulation results and box plots of ME are illustrated in Fig. 3. The comparison of the goodness-of-fit between the models was done by using ME, CD and in consideration of printed isoproturon profiles.

NJ’s and CB’s results using MACRO show a remarkably good fit for isoproturon concentration in soil 1993/1994 after modifying pesticide parameters which were derived from literature and not only from the Weiherbach data set (cal 2). This is reflected in the two statistical indices (ME and CD in Table 6) which nearly reached an optimal value. MACRO (IB) could also predict isoproturon behaviour in soil well. This is indicated by the statistical indexes. LEACHP, WAVE and GLEAMS described fate and transport of isoproturon in a satisfying way. The results from the uncalibrated simulations with MACRO (CB and NJ) using the pesticide parameters estimated directly from the laboratory results given in the Weiherbach report are worse. The worst prediction was made with the SIMULAT model.

3.1.4. Blind simulation 1995

For 1995 only results of ‘calibrated’ simulations are reported. Calibration of hydraulic parameters using measurements of bromide concentration and soil moisture of 1993/1994 (model run ‘cal 1’) and in some cases changing of pesticide parameters (model run ‘cal 2’) were performed. A further calibration was not possible because the data of 1995 were not available for participants of the modelling exercise. As a result of the different environmental conditions (study period in spring 1995 vs. autumn/winter 1993/1994) some modellers, increased the degradation rates for 1995 compared to 1993/1994 (CB
Fig. 3. Box plots of model efficiencies for calculating isoproturon 1993/1994.
and IB with MACRO, GLEAMS). Others used the same degradation and sorption parameters as for the simulation period 1993/1994 (see Table 1).

3.1.5. Soil moisture 1995

Model predictions of the soil moisture in 1995 are worse than the results for 1993/1994. The initial water content was not given for the simulation period 1995. Therefore one reason for the bad predictions could be the initial conditions chosen by the model users. The best fit for soil moisture was obtained with SIMULAT (see Fig. 4) and GLEAMS. Fig. 5 summarises the box plots of the ME’s of all sampling dates. The mean ME of SIMULAT and GLEAMS are $-3.248$ and $-3.255$ (model 1993/1994 ME = $0.113$ and $-0.461$). WAVE, LEACHP and MACRO (NJ) show similar ME between $-6.444$ and $-7.818$. The other two MACRO users (CB, IB) did not predict the water content in soil correctly. This is indicated by an ME of $-15.171$ and $-15.955$. The ME box plots of MACRO (IB) also show the biggest range in comparison to all other models.

3.1.6. Bromide concentration in soil 1995

Transport of bromide in soil of Field Plot VIII was very fast compared to 1993/1994. Nearly all of the applied 150 kg ha$^{-1}$ of bromide was leached $>95$ cm during 6 weeks. All models had difficulties in predicting the behaviour of the tracer in 1995, which is reflected in low mean ME in and dispersed ME shown in box plots of Fig. 6. LEACHP gave the best prediction of bromide concentration in soil (see Fig. 7) with an ME of 0.101, followed by WAVE (ME = 0.078), MACRO (NJ) (ME = $-0.037$) and MACRO (CB) (ME = $-0.312$). MACRO (IB) and SIMULAT show the worst results reflected in low model efficiencies of $-1.323$ and $-1.493$. ME was not calculated for GLEAMS because model output could not be compared with the measurements. The user made a long-term simulation (1993–1995) including both bromide applications. This is reflected in two bromide peaks for simulation period 1995, because bromide applied 1993/1994 did not leach completely out of the monitored soil profile until the second tracer application in 1995.

3.1.7. Isoproturon concentration in soil 1995

Table 7 shows that the goodness-of-fit coefficients calculated for 1995 are generally better than those for 1993/1994, listed in Table 6. MACRO (IB, cal 2) gave the best
Fig. 4. Comparison of soil moisture simulated with calibrated model SIMULAT with the measured in the soil profile at Weiherbach on four days 1995. This model gave the best description of soil moisture for the simulation period (11/5/95–23/6/95).
Fig. 5. Box plots of model efficiencies for calculating soil moisture content 1995.
Fig. 6. Box plots of model efficiencies for calculating bromide concentration in soil 1995.
prediction of isoproturon in soil. Fig. 8 shows the simulation results with MACRO (IB) in comparison to the measured herbicide concentration in soil. This is reflected in all statistical coefficients (ME = 0.728, CD = 0.843). The results of simulations with MACRO (CB), WAVE and GLEAMS also show a satisfying fit for isoproturon concentration in soil. Box plots of ME show that the results of MACRO (CB and IB, cal 2), and GLEAMS and WAVE are less variable in comparison to those of all other models (Fig. 9).

Fig. 7. Comparison of bromide content simulated with calibrated model LEACHP with the measured bromide distribution in the soil profile at Weiherbach on four days 1995. This model gave the best description of bromide concentration for the simulation period (11/5/95–23/6/95).

Fig. 8. Comparison of isoproturon concentration simulated with calibrated model MACRO IB with the measured in the soil profile at Weiherbach on four days 1995. This model gave the best description of isoproturon concentration for the simulation period (11/5/95–23/6/95).
Fig. 9. Box plots of model efficiencies for calculating isoproturon concentration in soil 1995.
MACRO (IB, cal 1) using the same pesticide parameters for the spring experiment 1995 as for the experiment in winter 1993/1994, LEACHP and MACRO (NJ) could not predict the isoproturon concentration satisfactorily. The worst simulation was made with SIMULAT as the model user did consistently stick to the laboratory derived input parameters.

3.1.8. Simulations with the consensus parameter set

Computer runs with the parameters of the consensus parameter set were made with GLEAMS, MACRO (IB and CB) and SIMULAT. Statistical coefficients calculated from isoproturon predictions are reported in Table 8 for the simulation period 1993/1994 and in Table 9 for 1995.

3.1.9. Isoproturon concentration in soil 1993/1994

Nearly all models using the consensus parameter set show smaller deviations from measurements than the uncalibrated simulations using parameters estimated from the original Weiherbach data set (simulation runs ‘cal 1’) without any guidance by the data providers (compare statistical coefficients ME and CD in Tables 6 and 8). Despite the different model concepts of water and matter transport (capacity vs. Richards’ equation vs. macropore model) the models obtained similar results for the calculation of the isoproturon concentration in soil. This demonstrates that the choice of pesticide parameters which are the most sensitive, overrides the model differences. Therefore the differences between the calculated mean ME’s are relative small for all four simulations (between 0.199 and 0.486). The other statistical coefficients (CD = 0.869) indicates that IB with MACRO gave the best prediction of isoproturon behaviour in soil, too. Box plots given in Fig. 10 also confirm the best prediction of MACRO (IB) as the range of the

<table>
<thead>
<tr>
<th>Model</th>
<th>ME (best = 1)</th>
<th>CD (best = 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MACRO (CB)</td>
<td>0.268</td>
<td>0.702</td>
</tr>
<tr>
<td>MACRO (IB)</td>
<td>0.486</td>
<td>0.869</td>
</tr>
<tr>
<td>SIMULAT (KA)</td>
<td>0.275</td>
<td>0.769</td>
</tr>
<tr>
<td>GLEAMS (IB and SR)</td>
<td>0.200</td>
<td>0.697</td>
</tr>
</tbody>
</table>

Table 8

<table>
<thead>
<tr>
<th>Model</th>
<th>ME (best = 1)</th>
<th>CD (best = 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MACRO (CB)</td>
<td>−0.836</td>
<td>0.316</td>
</tr>
<tr>
<td>MACRO (IB)</td>
<td>0.032</td>
<td>0.088</td>
</tr>
<tr>
<td>SIMULAT (KA)</td>
<td>−1.311</td>
<td>0.280</td>
</tr>
<tr>
<td>GLEAMS (IB and SR)</td>
<td>−0.443</td>
<td>0.432</td>
</tr>
</tbody>
</table>

Table 9
Numerical comparison of model predictions: isoproturon concentration in soil of Field Plot VIII 1995 (consensus parameter set) (goodness-of-fit statistics)
Fig. 10. Box plots of model efficiencies for calculating consensus parameter set isoproturon concentration in soil 1993/1994.
Fig. 11. Box plots of model efficiencies for calculating consensus parameter set isoproturon concentration in soil 1995.
Model efficiencies calculated for each sampling date is the smallest one. SIMULAT and MACRO (CB) show similar simulation results indicated by the statistical coefficients in Table 8 and the box plots in Fig. 10 (mean ME are 0.275 and 0.268). The statistics show the worst predictions for GLEAMS but the values differ only slightly from the other models, e.g. ME = 0.199 and CD = 0.697.

3.1.10. Isoproturon concentration in soil 1995

The agreement between model predictions and measurements are less good for the simulation period 1995 (see Fig. 11). The decision which model gave the best simulation is difficult using the statistical parameters alone. The result depends on the chosen coefficient (ME or CD, see Table 9). A visual comparison of the results show, that GLEAMS gave the best prediction of isoproturon transport and decay. The simulation results of MACRO (IB and CB) show similar agreement with measurements which can be seen in the statistical coefficients. SIMULAT gave the worst prediction of isoproturon because the fast transport in soil could not be simulated without the macropore options of this model.

4. Discussion

NJ used another site than Field Plot VIII for estimation and calibration of hydraulic parameters for MACRO. This may explain why the calculation of soil moisture 1993/1994 with the calibrated model is worse compared to those of other MACRO users. But it is also shown that model predictions with hydraulic parameters estimated from a site with soil texture similar to Field Plot VIII were better for 1995 than those of all other MACRO users. The calculated bromide concentration corresponds relatively good to measurements in both simulation periods in comparison to all other models using model default values. Degradation parameters estimated from the laboratory experiments gave only bad simulation results. After optimising the pesticide parameters the model predictions agree very well with the measurements from 1993/1994, but not with the measurements from 1995.

After calibrating the hydraulic parameters of MACRO, CB achieved the best description of the water and bromide content in soil for 1993/1994. For 1995 he achieved only moderate results. Simulation results of isoproturon with calibrated pesticide parameters show best agreement with measurements 1993/1994 and also one of the best predictions in 1995. Considering all parameters which should be calculated, CB achieved the best simulations using the MACRO model.

IB used an older version of MACRO (3.1). Lack of calibration of the hydraulic parameters (except for the saturated hydraulic conductivity) is reflected in worse description of soil moisture and bromide concentration. As an explanation for the good agreement between predicted and measured isoproturon concentration in soil the choice of a higher saturated conductivity than measured, a lower sorption coefficient than measured and a faster degradation in 1995 than measured can be given. Modeller experience, the time available to get acquainted to the data set, and time available for the calibration had the main influence obtaining good simulation of isoproturon behaviour.
GLEAMS shows satisfying calculations of water content, bromide content and isoproturon transport and degradation for both years. In spite of the fact that GLEAMS is a capacity model, ME calculated for soil moisture are relatively good in comparison to other models using Richards equation. Nevertheless, the output data reveal that GLEAMS did not predict real hydraulic dynamic in soil. By using a maximal water content as input parameter similar to the mean water content measured in the soil during the simulation period, a good ME was achieved as changes in the water content in the field were small. The good predictions of isoproturon behaviour can be explained with the choice of realistic sorption and degradation parameters that deviate from the measurements in the laboratory.

SIMULAT gives good simulations of water 1993/1994 and 1995 and of bromide 1993/1994. Bromide transport 1995 and isoproturon behaviour for both periods could not be simulated in a satisfying way. SIMULAT was the only model which used degradation parameters that were estimated directly from the laboratory data and without further calibration. Presumably the use of the macropore option in SIMULAT together with more realistic sorption coefficients would have supplied better predictions of the behaviour of isoproturon and bromide.

Predictions of WAVE and LEACHP of soil moisture can be judged as acceptable in comparison to other models without further calibration of hydraulic parameters. WAVE and LEACHP adequately described the isoproturon and bromide concentrations in the soil for both simulation periods. Although on the one or other occasion other models gave better results, WAVE and LEACHP simulations were consistently good. It must be mentioned that the degradation parameters were calibrated with measured data from the field experiment in 1993/1994.

A satisfying description of the water content or the bromide concentration in soil in 1993/1994 was not achieved using PELMO (except PELMO run 3 and 4). The simulation results reflect the difficulties of capacity models like PELMO to describe the hydraulic dynamics in soil (see remarks on GLEAMS). A comparison with other models concerning the predictability of the hydraulic situation in 1995 or pesticide degradation was not possible because only simulation results of bromide and soil moisture of 1993/1994 were available.

A comparison of models according to their ability to predict the fate of pesticides as described so far was difficult because the simulation results did not only represent the quality of the model concepts but also the subjectivity of the model user to estimate the required input parameters. A major difference was also the extend of calibration for the model-user-run combinations. There are many examples in the literature of the affect of different users of a model on the results of simulations (Botterweg, 1995).

5. Conclusions

The most striking points of the modelling exercise were the diversity of parameters estimated by different users from the same basic data set and the problems in principal to simulate the field behaviour using laboratory derived pesticide parameters.

As described also by Boesten (2000) for a Dutch data set with a sandy soil, the overwhelming influence of the individual user on the model results was remarkable for
the Weiherbach data set. Although extensive and detailed laboratory measurements on the pesticide behaviour in the same soil were available, it was not possible to estimate a parameter combination from the laboratory data to describe the field behaviour of isoproturon satisfactorily. Only the consideration of field data and literature data from outside the Weiherbach project or calibration to the field results of the experimental period 1993/1994 did improve the simulation results significantly. Even the consensus parameter set, which was generated from the laboratory experiments after the first simulation results had become available, gave worse results than the parameters obtained by calibration to the field data or expert judgement.

It has to be kept in mind that the author of the consensus parameter set (Gottesbürren) tried to consider the information in literature while staying inside the range of the data generated by the Weiherbach group. For example a $K_{OC}$-value of 119 l kg$^{-1}$ was taken for isoproturon from a desorption experiment, which was more in line with literature values than the $K_{OC}$-value of 220 l kg$^{-1}$ from the adsorption/desorption experiments.

The results are contradictory to a modelling philosophy that assumes if enough information from accompanying laboratory experiments is available for the behaviour of a pesticide in a specific field can be simulated satisfactorily. Additional information from field studies improved the modelling results considerably especially for the ‘blind simulation 1995’, which raises some doubts on the exclusive use of laboratory parameters.

Good predictions of bromide and isoproturon concentration in one experimental period (e.g. 1993/1994) by a model did not imply a good agreement between simulation results and measurements in the second period 1995. As explanation an accelerated transport through macropores can be supposed for spring 1995 which could have occurred initially in the dry soil. In addition the question might rise — “Are the models adequate to simulate pesticide behaviour during autumn and winter as most models have been developed and tested under spring/summer conditions?” Effects of cultivation can additionally cause different transport behaviour of matter in soil. This fact could also explain why model calibration of hydraulic parameters with data from 1993/1994 does not imply a good prediction for 1995.

Model users who estimated degradation parameters directly from laboratory measurement did not gain satisfying results for 1993/1994 and for 1995, e.g. SIMULAT and uncalibrated MACRO (CB and NJ). But good predictions were possible after changing half-lives and sorption coefficients to realistic values as reflected by literature — CB and NJ obtained good predictions with MACRO (cal 2) for 1993/1994. For 1995 all model users except KA in SIMULAT decreased half-life values in comparison to 1993/1994.

SIMULAT, which calculated water content and bromide transport 1993/1994 very well, did fail in calculating the behaviour of isoproturon. The influence of sorption and degradation parameters on the prediction of pesticide behaviour was greater than the influence of water content or the transport in soil. Other models, e.g. MACRO (IB) show a good prediction of isoproturon transport in both years but simulations results of water content were not satisfying.

In spite of the fact that all MACRO users took similar model ‘consensus’ parameters from the consensus parameter set, the simulation results were different. Different initial
parameters as water content can be mentioned as an explanation for the discrepancies. For the simulation period 1993/1994 all models using the consensus parameter set showed similar results because phenomena only played a minor role. In the year 1995 the chosen transport parameters did have a great influence on the simulation results. This could explain why SIMULAT gave worse predictions compared to MACRO. The MACRO users did activate the macropore sub-model, whereas the SIMULAT user did not.

The direct model comparison was only possible with the defined input and model parameters. Otherwise the subjective influence of the model user was much greater than the difference between the models (see Boesten, 2000).

Additionally, a test of sub-models implied in complex models could have been useful. A comparison of simulation results, e.g. with and without plant uptake, macropore sub-model or temperature influence on degradation can show why a model gives better results than others. A step-by-step validation parallel with defining model parameters and initial values could be useful. The consensus parameter set described in this article was a first step but others should follow.

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References


