Simulation of soil water, bromide and pesticide behaviour in soil with the GLEAMS model

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Abstract

The GLEAMS model predicts runoff, percolation and soil and chemical losses at the edge of a field and from the root zone. The objective of this study was to test the performance of the GLEAMS model against three observed data sets from different parts of Europe. Three users tested the model independently, i.e. parametrized the model without discussion with the other users. Both uncalibrated and calibrated results are presented. Furthermore, the pesticide sub-model was parametrized according to proposals of the supplier of the measurement data. The test was focused on soil moisture, tracer (bromide) and pesticide movements in soil columns. The results show that GLEAMS soil moisture predictions appear to react too rapidly to wet and dry periods, resulting in a rapid change of soil moisture between field capacity and wilting point. Incomplete simulation of soil water dynamics seems to be the main reason for underestimation of tracer movement in soil. In addition, mismatches in soil pesticide concentrations might be caused by incorrect prediction of degradation processes. The results of the independent users differed considerably from each other, both in uncalibrated and in calibrated results, due to different interpretation of the measured data.

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1. Introduction

When assessing the environmental fate of plant protection products, e.g. in authorisation procedures, model calculations and estimates could provide a less
constrained and less expensive complementary approach to cover the large variation in
local land-use, management, as well as local natural conditions compared to experimental
studies. Currently, several models describing pesticide leaching are available, and their
possible suitability in the registration process was reviewed and reported by Regulatory
Modelling Working Group on Surface Water Models of FOCUS (FOCUS Leaching
Modelling Workgroup, 1995; FOCUS Soil Modelling Workgroup, 1997).

Before any model or models can be selected and approved for use as tools in the
pesticide registration process, their applicability and validity for the targeted purposes
should be tested and different models describing the same soil-water-atmosphere-plant
processes should be compared (Vanclooster et al., 2000). An important topic is to define,
for any potential model, its possible field of application in the registration process.
However, only very few model comparisons have hitherto been reported.

The aim of the mathematical modelling group of COST Action 66 has been to perform a
model evaluation and comparison study by testing different pesticide simulation models
using four common, high-quality experimental data sets.

The objective of this paper is to present the performance of the GLEAMS model
(Leonard et al., 1987) in predicting soil temperature, soil moisture, water percolation, and
the mobility of a tracer and selected pesticides under varying conditions. The
performance of GLEAMS is tested against three different observed data sets. In addition,
the modelling results obtained by three independent model users testing GLEAMS against
one data set (Vredepeel) were used to report the problems due to parameter estimation
difficulties.

2. Material and methods

The GLEAMS model (version 2.10) was tested against three observed data sets,
Vredepeel, Tor Mancina and Weiherbach, all of which are described in detail in this
volume.

The Vredepeel data originates from an experimental study launched to collect a good-
quality data set to test the PESTLA model (Boesten, 1993), which has been used in the
Netherlands in the pesticide registration process. A detailed description of the Vredepeel
data is given by Boesten and van der Pas (2000).

The Tor Mancina data set is the result of a 3-year lysimeter experiment carried out near
Rome (Italy), and aiming to assess the risk of groundwater contamination from some
herbicides commonly used in the Mediterranean area (Francaviglia and Capri, 2000). The
model output variables reported in this study were water percolation, bromide leaching
and the occurrence of metolachlor residues in leachates. All parameters refer to two
irrigation treatments (IRR2 > IRR1) which are used to evaluate the effects of different
water supplies.

The Weiherbach data set for pesticides was collected between 1993 and 1995 in south-
western Germany. Measurements of bromide and herbicide behaviour in soil were carried
out in a field plot, in small lysimeters and in the laboratory. The field experiments were
carried out during a winter period and two spring/summer periods. A detailed description
is given by Schierholz et al. (2000).
2.1. The GLEAMS model

The GLEAMS model (Groundwater Loading Effects of Agricultural Management Systems) is an extension of the CREAMS model (Knisel, 1980), which was developed in the United States in the late 1970s to predict non-point source losses of pollutants and to evaluate and compare agricultural management practices. CREAMS and GLEAMS are management oriented, field-scale mathematical simulation models, which predict runoff, percolation and soil and chemical losses at the edge of a field and from the root zone.

In the present version 2.10 of GLEAMS, most of the hydrology and erosion components are still the same as in the original CREAMS model. In the first version of GLEAMS the major modification was that it considered the vertical flux of pesticides into, within and through the root zone (Leonard et al., 1987). The major modifications included in version 2.10 consist of new nitrogen and phosphorus components and new options to estimate potential evapotranspiration. A short description of the hydrology, erosion and pesticide sub-models is given here.

The computation of the field-scale water balance includes models for surface runoff, infiltration, soil water movement and evapotranspiration. The surface runoff is predicted to the soil water content and is based on the water holding capacity of the soil. Calculation of the maximum retention is based on the SCS curve number method. The soil water balance considers both soil evaporation and plant transpiration, and the potential evapotranspiration can be estimated optionally by the Priestly–Taylor method (Priestly and Taylor, 1972) or by the Penman–Monteith method (Penman, 1948; Monteith, 1965; as described in Jensen et al., 1990). The prediction of soil loss is based on the Universal Soil Loss Equation (USLE), as described by Wischmeier and Smith (1958, 1978). Detachment of soil particles is described by a modified USLE (Foster et al., 1977) and the sediment transport capacity by the Yalin sediment transport equation (Yalin, 1963).

In the pesticide module the partitioning of the pesticide between the aqueous and solid phase at equilibrium is calculated using a linear adsorption isotherm. The model assumes a non-ionic pesticide and the adsorption occurs on organic carbon only. The adsorption coefficient $K_d$ is calculated from the adsorption coefficient for organic carbon, $K_{oc}$. The maximum concentration in the water phase is limited by the water solubility of the pesticide.

In addition to the pesticide directly reaching the soil surface during application, the amount of the pesticide in the surface layer of the soil is increased by wash off from foliage, and the total pesticide amount in the soil and foliage is reduced due to biological and chemical degradation. The overall rate of pesticide degradation is described by a first-order rate equation, e.g. in the soil

$$C_{soil}(t) = C_{soil}(0) \exp \left( -\frac{0.693t}{t_{1/2}} \right),$$

where $C_{soil}(t)$ is the pesticide concentration in the soil at time $t$, $C_{soil}(0)$ the initial pesticide concentration and $t_{1/2}$ the half-life of the pesticide in the soil. A different half-
life is considered for pesticide degradation on the foliage. Volatilisation is not included in the model.

A certain amount of pesticide percolates with the water flux to the lower soil layers and finally leaves the deepest layer (below the root zone). The amount of pesticides in soil is also exposed to plant transpiration and to the transport induced by water evaporation. The remaining pesticide on the soil surface is subject to removal by surface runoff and sediment loss due to erosion. In CREAMS/GLEAMS it is assumed that the topmost centimetre of the soil supplies effectively pesticide to the flow. In this soil mass the quantity of pesticide is the product of the runoff-available concentration, \( C_{av} \), and an extraction coefficient \( B \). Since it is assumed that the pesticide equilibrates instantly between the soil mass and the overland flow, we have

\[
C_w + C_s B = C_{av} B. \tag{2}
\]

Together with the sorption isotherm this allows calculation of the concentration in soil and water as a function of \( C_{av} \) at every time step (day). In GLEAMS, the extraction coefficient \( B \) is modelled as a function of the adsorption coefficient \( K_d \) and varies from 0.1 to 0.5 g ml\(^{-1}\) (Leonard et al., 1987).

Four methods for pesticide application are implemented in the model: (1) surface application: the pesticide is mixed into the surface layer (defined as the top 1 cm layer); (2) incorporation: the pesticide is mixed into the topsoil down to a given mixing depth; (3) injection: the pesticide is mixed into the soil layer defined by the injection depth; (4) chemigation: pesticide application with irrigation. The uppermost 1 cm soil layer contributes to the pesticide amounts in runoff. A more detailed description of the model can be found in Knisel (1980) and Leonard et al. (1987).

### 2.2. Driving variables and parametrization

GLEAMS requires several meteorological data series for each simulated year: daily values for precipitation and mean air temperature, and additionally monthly values for maximum and minimum air temperature, solar radiation, wind speed and dew-point temperature.

In this paper only the estimation of the most relevant parameters is described: soil texture, hydraulic conductivity, porosity, field capacity, wilting point, pesticide degradation half-life and the adsorption coefficient. Parameter estimation was a two-step process: (1) with no calibration (2) with calibration. The modelling procedure is described in detail in this volume by Vanclooster et al. (2000).

The parameter estimation was based on three main sources of information: measurements or calculations based on measurements, the GLEAMS manual or other literature sources, and expert assessments.

#### 2.2.1. Vredepeel

The meteorological input data were derived from weather stations located less than 30 km from the experimental field.

The simulated soil layers were determined according to the observations: 0–30, 30–60, 60–90 and 90–120 cm. The GLEAMS model automatically divides the simulated profile
into 10 layers, the depths of which are set automatically, in the present case resulting in the following: 0–1, 1–10.7, 10.7–20.3, 20.3–30, 30–45, 45–60, 60–75, 75–90, 90–105, and 105–120 cm.

The Priestly–Taylor equation was used to estimate potential evapotranspiration, and the initial soil water content was set at 100% of plant available water at the beginning of the simulation period (end of November).

For this data set three different GLEAMS users (User 1, User 2, User 3) estimated hydrological and pesticide parameters independently in the two-phase process (uncalibrated and calibrated). After compiling all the results the provider of the observed data also provided his estimates for the pesticide parameters (Boesten and van der Pas, 2000). Soil textural composition, organic matter content, bulk density and hydraulic conductivity were provided to the users. Several methods were used to estimate field capacity, wilting point and porosity: a pedo-transfer function proposed by the British Soil Survey and implemented in the LEACHW model (Hutson and Wagenet, 1992), direct observations, and literature values given in the GLEAMS database. The values selected by different users for hydraulic conductivity (cm h$^{-1}$), field capacity (cm$^3$ cm$^{-3}$) and wilting point (cm$^3$ cm$^{-3}$) for uncalibrated and calibrated model runs are reported in Table 1. User 1 did not perform any calibration for hydrological parameters, whereas the other users adjusted field capacity and wilting point using the estimation methods described above. As the moisture content was underestimated, User 2 increased the values for field capacity based on the fact that groundwater level in the region is supposed to be high and this gives rise to low tension.

Standard crop parameters (according to the GLEAMS manual) were used for the simulation. The chemicals (bromide and pesticides) were surface applied on bare soil. User 2 used exactly the given application rates (0.8 kg ha$^{-1}$ for bentazone and 3.3 kg ha$^{-1}$ for ethoprophos), whereas User 1 took into account recoveries observed immediately after application, and chose the rates 0.73 and 3.0 kg ha$^{-1}$ for bentazone and ethoprophos, respectively. User 3 estimated 10% dissipation due to the wind drift.

Table 1
The selected hydrological parameter values for hydraulic conductivity (RC, cm h$^{-1}$), field capacity (FC, cm$^3$ cm$^{-3}$) and wilting point (WP, cm$^3$ cm$^{-3}$) for uncalibrated and calibrated model runs by three independent users and the data provider$^a$

<table>
<thead>
<tr>
<th></th>
<th>RC$_1$</th>
<th>RC$_2$</th>
<th>RC$_3$</th>
<th>RC$_4$</th>
<th>FC$_1$</th>
<th>FC$_2$</th>
<th>FC$_3$</th>
<th>FC$_4$</th>
<th>WP$_1$</th>
<th>WP$_2$</th>
<th>WP$_3$</th>
<th>WP$_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uncalibrated User 1</td>
<td>7.69</td>
<td>10.52</td>
<td>10.52</td>
<td>10.52</td>
<td>0.21</td>
<td>0.13</td>
<td>0.12</td>
<td>0.13</td>
<td>0.04</td>
<td>0.03</td>
<td>0.03</td>
<td>0.04</td>
</tr>
<tr>
<td>User 2</td>
<td>6.9</td>
<td>11.4</td>
<td>10.4</td>
<td>10.4</td>
<td>0.15</td>
<td>0.18</td>
<td>0.10</td>
<td>0.10</td>
<td>0.02</td>
<td>0.03</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>User 3</td>
<td>9.15</td>
<td>10.3</td>
<td>10.3</td>
<td>10.3</td>
<td>0.16</td>
<td>0.16</td>
<td>0.16</td>
<td>0.16</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>Calibrated User 1</td>
<td>Uncalibrated</td>
<td>Uncalibrated</td>
<td>Uncalibrated</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>User 2</td>
<td>Uncalibrated</td>
<td>0.20</td>
<td>0.25</td>
<td>0.18</td>
<td>0.25</td>
<td>Uncalibrated</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>User 3</td>
<td>Uncalibrated</td>
<td>0.19</td>
<td>0.15</td>
<td>0.10</td>
<td>0.20</td>
<td>0.08</td>
<td>0.03</td>
<td>0.03</td>
<td>0.03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Data provider</td>
<td>RC = User 3, calibrated = uncalibrated, no data for FC and WP</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$^a$ The index (1–4) refers to the selected soil layers (0–30, 30–60, 60–90, and 90–120 cm).
resulting in the initial rates of 0.72 kg ha\(^{-1}\) for bentazone and 2.97 kg ha\(^{-1}\) for ethoprophos, respectively. The data provider proposed 0.63 kg ha\(^{-1}\) for bentazone according to the recovery 1 day after application, and 1.33 kg ha\(^{-1}\) for ethoprophos according to the recoveries observed 22 and 42 days after the application. This low recovery is due to high volatilisation of ethoprophos, which GLEAMS does not take into account.

Concerning the movement of bromide, three main parameters available from the Gleams literature were used to calibrate the model: Partition coefficient \(K_{oc}\), soil half-life, and crop uptake parameter. The uncalibrated and calibrated values selected by different users are shown in Table 2. Crop uptake of bromide was estimated by all users to be 0.18% of the application amount and only USER 3 changed this to 0.05% when calibrating.

In the case of pesticides, three users estimated the parameters for bentazone and ethoprophos independently in two steps, i.e. uncalibrated and calibrated simulations. Different users based the estimation of \(K_{oc}\) and soil half-life on observations, and also additionally on the Gleams database, which is based on the USDASCS database (USDASCS, 1972). Some of the users gave different values of half-life for each soil layer (Table 2). The water solubilities of these pesticides were taken from Wauchope et al. (1992). No uptake of pesticides by plants was assumed.

2.2.2. Weiherbach

The parameter values used are based on three main information sources: measurements or calculations, Gleams manual values and expert judgement. In the following the origin of the relevant parameter values is described.

The meteorological input data were either measured directly or calculated from measured values at the meteorological station of the Weiherbach catchment. Evapotranspiration in Gleams was calculated choosing the Priestly–Taylor equation. An initial value for the fraction of soil moisture at the beginning of the simulation period was estimated using measured soil moisture values and comparing them to the measured soil water contents at wilting point and at field capacity.

The maximum amount of soil layers in Gleams was used. The layers fed into the model were: 0–4, 4–16, 16–25, 25–35 and 35–100 cm. The model internally divided the soil layers further into the following final layers: 0–1, 1–4, 4–16, 16–25, 25–35, 35–48, 48–61, 61–74, 74–87, and 87–100 cm. The first four layers belong to the Ap horizon and the remaining layers to the C horizon. For these two horizons soil parameters were estimated separately. Soil porosity was calculated from the estimated bulk density; soil water contents at wilting point and field capacity were estimated from measured pF-curves; saturated conductivity was measured as well as the organic matter, clay and silt contents of the soil.

The plant parameters were estimated from measured reference crops at similar sites in the Weiherbach catchment. Gleams manual values were used for the soil evaporation parameter depending on soil texture (CONA) and for the SCS curve number corresponding to moisture condition II (CN2).

Erosion parameters were generally chosen so that the erosion risk was minimized, as no erosion was detected during the experimental period. No measurements were available
Table 2
The selected values for the partition coefficient ($K_{oc}$, cm$^3$ g$^{-1}$) and soil half-life ($t_{1/2}$, day) for uncalibrated and calibrated model runs for bromide, bentazon and ethoprophos by three independent users and the data provider

<table>
<thead>
<tr>
<th>Layer</th>
<th>$K_{oc}$ (ml g$^{-1}$)</th>
<th>$t_{1/2}$ (day)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Bromide</td>
<td>Bentazon</td>
</tr>
<tr>
<td>Uncalibrated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>User 1</td>
<td>All layers</td>
<td>0</td>
</tr>
<tr>
<td>User 2</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>50</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>50</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>50</td>
</tr>
<tr>
<td>User 3</td>
<td>1</td>
<td>All layers</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>400</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>100</td>
</tr>
<tr>
<td>Calibrated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>User 1</td>
<td>All layers</td>
<td>1</td>
</tr>
<tr>
<td>User 2</td>
<td>All layers</td>
<td>0.1</td>
</tr>
<tr>
<td>User 3</td>
<td>1</td>
<td>Uncalibrated</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Uncalibrated</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>100</td>
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<tr>
<td></td>
<td>5</td>
<td>100</td>
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<tr>
<td>Data provider</td>
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<td>96.1</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>96.1</td>
</tr>
</tbody>
</table>
for their estimation. A very small value for the drainage area was used due to the focus on a 21 m² field plot only.

For the specific surface area of clay particles the GLEAMS default value for kaolinite was used. The soil erodibility factor was calculated using a regression equation based on the organic matter content of the soil, the soil structure code and the soil profile permeability class, which were chosen from a GLEAMS manual table using the measured clay, silt and sand contents of the soil. The Manning’s $n$ for overland flow was chosen from a manual table giving values for a small grain crop with up-and-down slope planting and a dense vegetation stand.

All chemicals used were applied on the soil surface and an incorporation depth of 1 cm was assumed in the model. For the tracer bromide extremely high values were used for water solubility and soil half-life, whereas the sorption coefficient was set to zero. For the water solubility of the herbicide isoproturon a value ($65 \text{ mg l}^{-1}$) presented by the manufacturer was used. The half-life of isoproturon in soil is based on laboratory measurements of the degradation rate for the top soil. An average degradation rate of 0.03 per day was used to calculate a half-life of 23 days in the top soil in winter. Since GLEAMS does not include a temperature dependent degradation calculation, the half-life for the summer data series had to be estimated. Due to different environmental conditions in winter a three-fold higher half-life was assumed for this period compared to the summer period. The half-life for the summer period was therefore set to 8 days. The values for the foliage half-life were estimated from these soil half-life values using empirical factors recommended in the GLEAMS manual. For the sorption coefficient $K_{oc}$ a literature value of 91 cm³ g⁻¹ was used. For both bromide and isoproturon a low uptake by plants of 0.1 was estimated on a range from 0.0 to 1.0.

During calibration only one parameter was changed; the soil moisture content at field capacity. Instead of the rather high values determined by measurements (37.2% for the Ap horizon and 41.3% for the C horizon) a smaller value from a GLEAMS table was chosen (27% for both horizons). This value was chosen due to the texture class of the soil, which in turn was estimated using the measured clay, silt and sand contents of the soil.

2.2.3. Tor Mancina

Meteorological data were measured at a climatic station close to the lysimetric installation. Potential evapotranspiration was estimated according to Penman–Monteith, since this equation is more suitable for arid climates. The method requires some additional data inputs, i.e. mean monthly wind speed and dew-point temperature. Since the latter was not available in the data set, it was estimated using the Tetens method reported by Jensen et al. (1990).

Initial soil water content was set to 20% of the available water, since at sowing the soil was very close to the wilting point. Values given in the data set were used for field capacity and wilting point, whereas values of saturated conductivity were modified according to the minimum values reported in the model description for the corresponding soil class. This calibration was performed in order to obtain a simulated percolation as close as possible to the experimental data.
Specific LAI development curves were set for all crops, for two main reasons:

- broad bean and french bean crops are not included in the model; and
- standard values for soybean, winter wheat and corn are very low in comparison with common local data.

In the case of the movement of bromide, the following parameters available from the GLEAMS literature were used to calibrate the model: the partitioning coefficient $K_{oc}$ was set to 1 ml g$^{-1}$, soil half-life to 100 000 days, and crop uptake to 0.18% of the application rate.

Metolachlor was surface applied and the parametrisation was derived from the GLEAMS database. $K_{oc}$ was set to 200 ml g$^{-1}$ and the half-life to 90 days. No further calibration was made. No uptake of metolachlor by plants was assumed.

3. Results

3.1. Evapotranspiration

No actual measurements of evapotranspiration were provided in any of the data sets. However, in the Vredepeel data daily values for evapotranspiration estimated by the Makkink equation (see Feddes, 1987) were given. In GLEAMS either Priestly–Taylor or Penman–Monteith equations can be selected to calculate evapotranspiration. For the Vredepeel modelling Priestly–Taylor was selected. In Fig. 1 Makkink potential evapotranspiration is compared to actual evapotranspiration based on the Priestly–Taylor equation. When calculating the actual evapotranspiration, the soil moisture is a limiting factor resulting in much lower estimates particularly during the growing season and summer.

Fig. 1. Cumulative potential evapotranspiration calculated by the Makkink equation (thin line) (provided with the observations) and actual evapotranspiration calculated by GLEAMS using the Priestly–Taylor equation (thick line) for the Vredepeel data.
3.2. Water percolation

Water percolation through the root zone was tested against the Tor Mancina data set. Since the experimental data of treatment IRR2 were not significantly different from the IRR1 data, they have been considered as a single treatment in the comparisons. Fig. 2 shows the maximum and minimum values of water percolation of each sampling date, i.e. the maximum and minimum values selected among the four lysimeters. The vertical bars represent the calculated experimental error, which is equal to 10% as an average over all the experiments. Even after calibration, the model shows an earlier beginning of percolation, and from January 1994 up to the beginning of 1995 simulated data are lower than measured data. After that, GLEAMS overestimated the percolation systematically in both treatments.

3.3. Soil temperature

The overall behaviour of the calculated soil temperature was in relatively good agreement with the observed values in Vredepeel and Weiherbach (see Fig. 3). However, during certain peak (cold or warm) periods GLEAMS predicts somewhat more extreme values (low or high) compared to observed data. This can be seen particularly in the case of Weiherbach: the fluctuation of the predicted values was clearly sharper than in the observed data, and the peak low values were from 5 to 10°C lower in the simulated data than in the observed data.

3.4. Soil moisture

The differences in modelling soil moisture against the Vredepeel data set between different users were high in uncalibrated model runs particularly during the wet season.
Calibration clearly improved the results, and also brought the results by different users closer to each other. The model performance against the observed data was relatively good during the dry season (day 278), but during the wet season (days 103 and 474) the model had difficulties to match the higher observed values in deeper soil layers (60–90 and 90–120 cm, see Fig. 4).

According to this study, prediction of soil moisture with the GLEAMS model could only coarsely follow the measured fluctuations as can be seen in Fig. 5. GLEAMS allows the soil water content to vary only between the selected field capacity and the wilting point. However, as the observations clearly show, in wet conditions during autumn and winter the soil water content may often rise above field capacity towards saturation. Another feature in the calculated soil moisture is that it drops from field capacity to wilting point very quickly, and also increases as quickly after rainfalls. The continuous observations in the Weiherbach catchment data set show that the reactions are less sharp. This might result in problems when simulating chemical movements in soil.

Fig. 3. Measured (meas., thick line) and simulated (sim., thin line) soil temperature at Vredepeel (soil depth 2.5 cm) and at Weiherbach (soil layer 32 cm for measured and 25–35 cm for simulated results).
In the Weiherbach data set a better description of the measured moisture contents and bromide behaviour in soil was achieved using a lower value for the moisture content at field capacity (gained by calibration) than the rather high value from the laboratory study (see Figs. 5 and 6). The use of the value derived from laboratory measurements resulted in overpredicted soil moisture levels and in retarded bromide leaching in comparison to the measurements.

In conclusion it can be stated that both modelled daily values and frequent observations indicate that the soil water content shows high variation and rapid fluctuation. This means that infrequent observations (as in the Vredepeel data set) are difficult to use as test data for models with daily output.

Fig. 4. Observed, uncalibrated and calibrated simulated soil water content (cm$^3$ cm$^{-3}$) at the depths 0–30, 30–60, 60–90 and 90–120 cm for the Vredepeel soil by three independent model users on days 103 (a and b), 278 (c) and 474 (d).
3.5. Bromide concentration

The upmost surface layer in GLEAMS is fixed to 1 cm and in the observed data the surface measurements were performed from a thicker layer (e.g. 0–4 cm in Weiherbach). This fact makes the comparisons difficult in this layer. However, it appears that GLEAMS predicts higher peak values in the surface layer immediately after application (Fig. 7).

In deeper layers down to 50 cm the predicted peak values are in rather good agreement with the observed values, but generally the decrease of bromide concentration is faster in the observed data than in the predicted data (see Fig. 6). This is probably due to inaccuracies of water movement modelling, which can be seen in the rather poor agreement in soil moisture results. Other possible reasons are inaccuracies in plant uptake.
of bromide, and the lack of dispersion and diffusion descriptions in the model. In layers beneath the active root zone (>35 cm), the modelled results do not behave very rationally. Although the fit to the observed values is relatively good, the unexpected increases between the two applications in the Weiherbach calculations are an indication of problems in the model structure.

For the Tor Mancina data set the differences between modelled and observed data can partly be explained by differences in percolation modelling (see Fig. 8), but in this case the GLEAMS results show good agreement in the final part of the experiment.

3.6. Pesticide concentrations

In this study four pesticides were tested: bentazone and ethoprophos in Vredepeel, isoproturon in Weiherbach and metolachlor in Tor Mancina.

For the Vredepeel data the most significant feature for both bentazone and ethoprophos is the relatively high variation of the results between different users (Figs. 9 and 10). Very often two- or three-fold differences were reported. In extreme cases the results by different users differ more than an order of magnitude from each other. For bentazone (Fig. 9) the calibrated model results were relatively good on the first observation date (day 103 after application), whereas later (day 278) some of the users predicted too high values in all soil layers, while one user predicted too low values in deeper soil layers. On the last observation day two users predicted approximately zero values, which fit well to the observations. Using the parameters estimated by the data provider did not give rise to better results than those of the best fitting user (USER 3).

The general feature for all ethoprophos predictions is that the model simulates too high values, except in the surface layers on days 103 and 278 (Fig. 10). Even considering the information of the data provider, in which the volatilisation of ethoprophos was taken into account, did not improve the predictions.
The behaviour of the relatively mobile pesticides bentazone and isoproturon was very similar to the bromide behaviour: the peak values were predicted relatively well, but the decrease in concentrations was slower in the calculated results. However, the infrequent observations in the Vredepeel data did not allow good comparisons over time. Furthermore, as in the case of bromide, the prediction in the layer beneath the root zone was poor.

Fig. 6. Simulated uncalibrated (thin solid line), simulated calibrated (thick solid line) and observed (dots) bromide concentrations in seven different soil layers at Weiherbach.
At Weiherbach the model followed the peak values of isoproturon immediately after the application rather well (Fig. 11), but the decrease in the pesticide content was too slow compared to the observations. Moreover, the fit of the model was better in upper layers compared to the lower soil layers. The degradation rate of pesticides did not change along with changing soil temperature or humidity in the model. Degradation was controlled by the given initial half-life value, which had to be estimated from laboratory experiments. The overestimation of degradation and underestimation of isoproturon concentrations in summer 1995 was most probably due to an inaccurately estimated
initial half-life for this period. The half-lives from the data provider were clearly higher for both observation periods (80 days for the winter period 1993/1994 and 37 days for the summer period 1995) than those estimated from the field data. These values resulted in a better estimation of the peak values for isoproturon in the summer period 1995, especially for the upper layers. On the other hand a much larger tailing of the isoproturon contents was simulated for each layer, which is not consistent with the observed behaviour in soil. It seems that either the laboratory values do not describe correctly the degradation in the field, or that the model does not account correctly for all the processes involved in calculating degradation. For instance, the model does not take into account the influence of soil moisture on degradation and the soil temperature is only indirectly taken into account. The results of total mass of isoproturon in the soil profile as a function of time (Fig. 12) support this conclusion. The degradation in the winter period is too slow for both parameter sets and the uncalibrated parameter set clearly results in an over predicted degradation during summer.

GLEAMS did not simulate the occurrence of metolachlor in leachates with the uncalibrated parameters derived from the GLEAMS data set. No further calibration was made, since this would have meant forcing the model to use unrealistic data. The input parameters derived from the data set would not improve the model performance, either.

4. Discussion and conclusions

The GLEAMS model is devoted to the simulation of chemical transfer in surface runoff and erosion at the edge of a field and in percolation water out of the root zone. Its use in
predicting pesticide movements in lysimeters or in small plots (e.g. Weiherbach 21 m²) might lead to inaccuracies in predicting these components on this scale. For example, GLEAMS induces surface runoff whenever there is excessive water on the soil surface, whereas lysimeters are usually constructed to prevent surface runoff. Thus, the test data used in this exercise may not be the best possible to show the suitability of such a model and on the other hand GLEAMS is perhaps not the most suitable model to describe pesticide movement in lysimeters and small plots.

The simulated soil temperatures fit reasonably well with the observed temperatures. In the case of evapotranspiration, no direct comparison can be made with GLEAMS calculations due to the lack of actual measurements. However, the problems after a

Fig. 9. Observed and calibrated model results by three independent users and the data provider for bentazone in the Vredepeel data set on days 103 (a), 278 (b) and 474 (c).
long dry period followed by irrigation (the Italian data set) show that in such extreme conditions the model cannot predict evapotranspiration correctly.

Being a capacity-type model, GLEAMS simulates changes in soil moisture which appear to be much too rapid compared with the observed values. During the wet season, or after rainfall events, GLEAMS sets soil moisture to the selected field capacity. It does not allow the moisture to increase above this value. Similarly, after rainfall, simulated soil moisture values quickly decreased to the selected wilting point. The observations, particularly from the Weiherbach experiment in Germany, show that the changes from field capacity to wilting point are not as rapid as those predicted by the model, and during a wet season soil moisture may increase above field capacity towards saturation. In fact, the GLEAMS model assumes that, when soil moisture is higher than field capacity, rapid percolation is always possible so that the daily moisture content never exceeds field capacity. Thus, it appears that this model is not suitable to describe saturated soil conditions and may only be used in well drained soils. Moreover, GLEAMS did not simulate correctly the percolation of water during the spring periods of 1994 and 1996 in the Italian data set. It is probable that the movement of water through the soil is not simulated correctly. In other words, the module for the redistribution of water through the soil profile is probably inadequate to describe local conditions, since it does not consider the possible occurrence of preferential or by-pass flows through macropores and soil cracks due to the soil texture (silty-clay loam). Furthermore, the model does not take into account the upward water movement by capillary rise. Some attempts to adapt GLEAMS to the Italian data have been made only for limited areas of the lower plain of the Po river, and for some typical crops (Morari and Giupponi, 1994).

The performance of GLEAMS can also be related to the difficulty of calibrating the parameters of some crops of the Italian data set (fodder bean and French bean), since they were not included in the standard database of the model.

The incomplete simulation of soil water movement dynamics appears to be the main reason for underestimation of bromide movement in soil. However, the mismatches in
pesticide concentrations in soil over time seem to be more due to incorrect degradation description than due to incorrect soil water prediction.

As discussed above, the GLEAMS model does not take into account preferential flow, which may however explain the occurrence of metolachlor in the observed leachates in Tor Mancina. In fact, some cracks were visible during the seed bed preparation in spring 1993, and additional cracks developed after every dry period during the experiment. Moreover, metolachlor was detected in samples rich in sediment, suggesting a rapid movement of water, solutes and soil particles with adsorbed herbicide through the soil layers.

One of the most striking conclusions based on this study is that the results of different independent users may differ so much from each other. This was particularly true for

![Diagram](image_url)

Fig. 10. Observed and calibrated model results by three independent users and the data provider for ethoprophos in the Vredepeel data set on days 103 (a), 278 (b) and 474 (c).
Fig. 10. (Continued)

Fig. 11. Simulated uncalibrated (thin solid line), simulated calibrated (thick solid line) and observed (dots) isoproturon amounts in different soil layers at Weiherbach.
uncalibrated simulation results. The calibration brought the results closer to each other, but still the differences were remarkably high. This means that (1) parameter estimation is difficult when it is mainly deduced from measured data, which different users interpret differently despite the relatively good quality of the data, and (2) the model is very sensitive to these parameters. In future, when testing models and not the capabilities of different users in parameter estimation, a full set of input parameters should be provided or recommended by the data provider to ensure the user-independent comparison of various models. Moreover, the model to be tested should be adapted to the local conditions to be described: in fact predictions cannot agree with observations if the model does not consider the key processes for a given situation.

Fig. 12. Total mass of isoproturon in profile (mg m\(^{-2}\)) as a function of time during the winter experimental period 1993/1994 (period 1) and the summer period 1995 (period 2): uncalibrated simulation (thin line with diamonds), simulation with parameters from the data provider (thin line with squares) and observed at Weiherbach (thick line with dots).
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