Comparison of the performance of pesticide-leaching models on a cracking clay soil: results using the Brimstone Farm dataset

Adrian Armstrong,*, Karin Aden, Nadia Amraoui, Bernd Diekkrüger, Nick Jarvis, Christophe Mouvet, Peter Nicholls, Caroline Wittwer

ADAS Research Gleadthorpe, Meden Vale, Mansfield, Notts NG23 9PF, UK
Institute of Geography and Geoecology, Technical University of Braunschweig, Langer Kamp 19c, 38106 Braunschweig, Germany
BRGM, Research Directorate, Avenue C. Guillemin, BP 6009, F-45060, Orléans Cedex 2, France
Geographische Institute der Universität Bonn, Meckenheimer Alle 166, D-53115 Bonn, Germany
Department of Soil Sciences, Swedish University of Agricultural Sciences, Box 7014, S-750 07 Uppsala, Sweden
IACR Rothamsted, Harpenden, Herts, AL5 2JQ, UK

Abstract

The leaching of the pesticide isoproturon from the macroporous clay soil at Brimstone Farm was modelled using four alternative models (MACRO, CRACK-NP, SIMULAT and PLM). Model results are presented for two test periods, the whole of one winter for which daily observations are available, and a short subset for which hourly data were presented. The best results are those given by MACRO with an expert user, although satisfactory results were also obtained from CRACK-NP and for the longer test period by PLM. SIMULAT was less successful in modelling the site because it did not include an adequate representation of the site hydrology, it was unable to predict the leaching of pesticide. MACRO was also used by a second modelling group who were less familiar with both the code and the site. Although the initial uncalibrated runs from this group were poor, the final calibrated results were almost as good as those derived by the ‘expert’ user. The simulations showed the difficulty of deriving adequate representations, even where relatively complete soil physical data are available. A shortcoming of the dataset provided was the lack of detailed soil moisture observations, particularly to define the initial conditions. From a well-monitored site,
many observations of site hydrology (water table position, drainflow and surface flow) were available, but significantly, fewer pesticide concentrations in either the soil or the discharges were available. Models could thus be evaluated only in terms of their ability to predict the magnitude and timing of major pesticide leaching events. © 2000 Elsevier Science B.V. All rights reserved.

**Keywords:** Model calibration; Macropores; Clay soils; Preferential transport; Isoproturon; MACRO; CRACK-NP; SIMULAT; PLM

### 1. Introduction

This paper presents a comparison of models applied to data from a structured clay soil within the context of the COST 66 Exercise: the comparison and evaluation of pesticide leaching models. The results of the applications are described and an evaluation is made of the models in terms of their ability to reproduce the observed hydrology of the site and the movement of the herbicide isoproturon to field drains.

Clay soils present a major challenge for pesticide leaching models (Armstrong et al., 1995). The presence of pathways for the preferential transmission of water and, with it, pesticide to the drainage system, can lead to the rapid transmission of pollutants to receiving surface water courses. However, clay soils represent only one set of conditions that might lead to preferential flow, and it is now recognised that preferential movement of water and solutes can occur under a wide range of conditions (Armstrong and Jarvis, 1997). About one-third of the land area of England and Wales can be classified as having soil with a significant potential for by-pass flow. The vast majority of these soils are drained where arable cultivation is practised (Brown et al., 1999).

#### 1.1. The Brimstone Farm dataset

Data from the Brimstone Farm site are reported by Harris et al. (2000) and Harris et al. (1994). From the extensive dataset two periods in the winter of 1990–91 were chosen for model evaluation:

- a short period (15 December to 15 January) during which detailed measurements of pesticide concentrations in the drainwater were available, and
- the whole of the winter period (October 1990 to March 1991).

Data were gathered for two plots: 6 and 9. These two plots varied in the efficiency of their drainage systems and in their agricultural management (Harris et al., 2000). Both plots had mole drains, which provided frequent (2 m spacing) shallow drains with a direct connection to the topsoil via vertical fissures (Spoor, 1994). Plot 6 was in a continuous cultivation cycle, and the residues were buried and incorporated by conventional moldboard ploughing. The herbicide isoproturon was applied in the autumn to a winter wheat crop. In contrast, Plot 9 was left fallow after burning of the crop residues and received no herbicide in the autumn. However, only one of the modellers chose to simulate Plot 9 due to the difficulty in determining initial isoproturon residue levels in the soil resulting from applications in previous year.
2. The models and modelling procedures

Four models were run for the Brimstone Farm dataset, MACRO, CRACK-NP, SIMULAT and PLM. The selection of models was the result of the COST66 group of modellers deciding which models were suitable for the modelling of the cracked clay soil. It was thus decided that the models that did not explicitly include a macropore component (GLEAMS, PELMO, PESTLA, PRZM-2 and WAVE) were not suitable for application to this dataset. The small number of models that were used and the few users in the exercise is a reflection of both the limited availability of models for the prediction of water and solute movement in macroporous soils, and their difficulty in use.

One model (MACRO) was run by two modelling groups independently, making five sets of model runs in all. Table 1 identifies the modelling groups involved. Following the agreed workshop protocols, (Vanclooster et al., 2000), and the procedure suggested by Armstrong et al. (1996), the initial model runs were attempted and calibrated (if necessary) using only the measurements of site hydrology. The models were then run with the pesticide component added, without additional calibration, and these were then evaluated.

2.1. MACRO

The dual-porosity MACRO model is a general purpose leaching model that includes the effects of macropores (Jarvis, 1994; Jarvis et al., 1994, 1995). It explicitly considers the macroporosity as a separate flow domain assuming gravity flow of water and a simple power law function for the conductivity. Solute movement in the macropores is assumed to be dominated by mass flow. The concentration of solutes in water entering the macropores at the soil surface is calculated using the ‘mixing depth’ concept, whereby the incoming rain perfectly mixes with the soil solution in a given depth of soil. Unlike the CRACK-NP model (Armstrong et al., 2000), MACRO also describes the movement of water through the soil matrix using Richards’ equation and of solutes using the convection–dispersion equation. Sorption is described with a linear isotherm, partitioning the sorption sites between the two domains. Degradation is calculated using first-order kinetics, with the possibility to specify different rate coefficients for both sorbed and solution phases, and in macropores and micropores. Version 4.0 of the model was used in this paper.

Table 1
Models and modelling groups participating in the modelling of the Brimstone Farm dataset

<table>
<thead>
<tr>
<th>Model</th>
<th>Institution</th>
<th>Modellers</th>
</tr>
</thead>
<tbody>
<tr>
<td>MACRO-User 1</td>
<td>SLU Uppsala</td>
<td>Jarvis</td>
</tr>
<tr>
<td>MACRO-User 2</td>
<td>BRGM</td>
<td>Amraoui, Wittwer, Mouvet</td>
</tr>
<tr>
<td>CRACK-NP</td>
<td>ADAS</td>
<td>Armstrong</td>
</tr>
<tr>
<td>SIMULAT</td>
<td>Univ. Bonn/BASF Aktiengesellschaft</td>
<td>Diekkrüger, Aden</td>
</tr>
<tr>
<td>PLM</td>
<td>RES</td>
<td>Nicholls</td>
</tr>
</tbody>
</table>
2.1.1. MACRO-User 1

The first MACRO user calibrated the hydrological components of the model. This strategy was adopted mainly due to the uncertainty with regard to the initial water contents at the site, which is especially critical for such short-term simulations, where the initial conditions may greatly influence the results. Four parameters (saturated hydraulic conductivity, macroporosity, macropore tortuosity and saturated conductivity of the matrix) were calibrated, largely against the measured drainflows, since the measurements of water table position were considered less reliable. Table 2 lists the resulting soil hydraulic parameter values used for the simulations presented here. With respect to the solute transport component, the model was first run without calibration in order to test the purely predictive ability of the model. Consequently, the parameter values were initially based on measured data (sorption $K_d$ values and half-lives) and default ‘library’ values. However, three parameter values (the mixing depth, the fraction of sorption sites in macropores, and the diffusion path length controlling mass exchange between the flow domains) were a priori changed from the default values based on the user’s familiarity with modelling similar soils. The values adopted (mixing depth: 1 mm; macropore sorption site proportion: 0.02; diffusion path length: 50 mm in the topsoil and 150 mm in the subsoil) may be considered informed expert choices. The values of diffusion path length chosen are similar to the values adopted by Armstrong et al. (1995, 2000) in the CRACK-NP model simulations. Subsequently the mixing depth was reduced to zero to improve the fit of the model to the observations.

2.1.2. MACRO-User 2

The second group using MACRO presented two sets of results from the MACRO model: those relating to an initial uncalibrated run, and the final calibrated run. The improvement between the two illustrates the need for calibration in such models. The modelling group attempted to use MACRO with a minimum of prior information and so started with the observed parameters provided by Armstrong (1995). They also started from a position of unfamiliarity both with the model and with the site. These are thus the only truly uncalibrated runs presented in this paper, as the other users all started from a

Table 2

Hydraulic parameter values in the MACRO simulations by User 1. (Detailed discussion of parameter meanings is given by Jarvis, 1994).a

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>$K_s$ (mm/h)</th>
<th>$K_{s(mi)}$ (mm/h)</th>
<th>$\theta_s$ (cm$^3$/cm$^3$)</th>
<th>$\theta_{s(mi)}$ (cm$^3$/cm$^3$)</th>
<th>$\theta_r$ (cm$^3$/cm$^3$)</th>
<th>$\Psi_{s(mi)}$ (cm)</th>
<th>$\lambda$</th>
<th>$D_{eff}$ (mm)</th>
<th>$n^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0–20</td>
<td>100</td>
<td>0.05</td>
<td>0.54</td>
<td>0.50</td>
<td>0.00</td>
<td>10</td>
<td>0.077</td>
<td>50</td>
<td>2</td>
</tr>
<tr>
<td>20–35</td>
<td>50 to 5</td>
<td>0.05</td>
<td>0.51</td>
<td>0.50</td>
<td>0.00</td>
<td>10</td>
<td>0.061</td>
<td>150</td>
<td>2</td>
</tr>
<tr>
<td>35–65</td>
<td>2</td>
<td>0.05</td>
<td>0.51</td>
<td>0.50</td>
<td>0.00</td>
<td>10</td>
<td>0.048</td>
<td>150</td>
<td>2</td>
</tr>
<tr>
<td>65–90</td>
<td>1</td>
<td>0.05</td>
<td>0.51</td>
<td>0.50</td>
<td>0.00</td>
<td>10</td>
<td>0.054</td>
<td>150</td>
<td>2</td>
</tr>
<tr>
<td>90–150</td>
<td>0.5</td>
<td>0.05</td>
<td>0.51</td>
<td>0.50</td>
<td>0.00</td>
<td>10</td>
<td>0.062</td>
<td>150</td>
<td>2</td>
</tr>
</tbody>
</table>

a $K_s$ — saturated hydraulic conductivity of macropores (mm/h); $K_{s(mi)}$ — saturated hydraulic conductivity of micropores (mm/h); $\theta_s$ — Saturated moisture content, total soil (cm$^3$/cm$^3$); $\theta_{s(mi)}$ — saturated moisture content, micropores (cm$^3$/cm$^3$); $\theta_r$ — residual water content (cm$^3$/cm$^3$); $\Psi_{s(mi)}$ — moisture tension for initiation of macropore flow (cm); $\lambda$ — pore size distribution index in Brooks–Corey equation; $n^*$ — pore tortuosity (dimensionless); $d_{eff}$ — effective diffusion path length (mm).
position of some prior knowledge. The first uncalibrated runs thus identify the degree to which the information provided was sufficient on its own for a successful model run. Calibration was performed using the longer test period, and the parameters that best fitted that period (Table 3) were then applied to the shorter period without further calibration. Despite starting from a position of low familiarity with both code and site, the group produced interesting results which fitted the observations moderately well.

2.2. **CRACK-NP**

CRACK-NP is a special-purpose model designed for cracking clay soils. It differs from other models in that it assumes water moves through the profile only in the macropores.
CRACK-NP has no component for the movement of water through the soil matrix, which is made up of peds, which absorb and desorb water and interact with the water moving through the surrounding macropores. A description of this model is given by Armstrong et al. (2000) and the parameters used (Table 4) were derived from the description of the soil of the site (Harris et al., 2000). The model was developed for the site, and has been shown to represent both the hydrology, and the movement of nitrate at the site (Armstrong et al., 1996). Parameters describing pesticide behaviour at this site (half-life and sorption) are available from the studies reported by Harris et al. (1994). The results presented here were thus derived from the five-stage validation procedure described by Armstrong et al. (1996).

2.3. **SIMULAT**

SIMULAT 2.3 (Diekkrüger et al., 1995; Aden and Diekkrüger, 2000) is a one-dimensional model of the transport and transformation of biodegradable substances (nitrate, pesticides) in the soil unsaturated zone. It contains sub-models for plant growth, run-off, evapotranspiration, heat flux in soil or water and matter transport, and includes, as an option, transport in the macropores. The model requires daily or hourly climatic data.

Water transport is solved by coupled partial differential equations (modified Richards’ equation), for which the retention and conductivity curves are required. The necessary parameters for the retention and conductivity curves after van Genuchten/Mualem were estimated from measurements (pF and corresponding water content) described by Armstrong (1995) using the SOPHY program available within SIMULAT (Diekkrüger and Arning, 1995). For Brimstone Farm, the simulated soil column was subdivided into compartments 2.5 cm thick from 0 to 20 cm and 10 cm thick layers from 20 to 200 cm depth. The internal model compartments represented four soil layers which were separately parameterised (Table 5). The saturated water content of the soil matrix was calculated from the total porosity minus stable drainable porosity.

A special version of SIMULAT (Diekkrüger, 1992) used the Hooghoudt drainage equation to calculate the rate of drain flow as a function of water table height (Hooghoudt, 1940; Ritzema, 1994) to represent the mole drainage system at Brimstone
Farm. A saturated conductivity of 10 cm per day was assumed. After calibration, the conductivity in the first 0–25 cm was reduced to 1 cm per day to initiate a higher macropore flow. A linear cascade model and no free drainage for macro pore flow were set as the bottom boundary. Lateral flow from macropores into the soil matrix was possible.

Water flow in the macropores is purely gravitational. Lateral infiltration into the matrix pores is computed by Darcy’s law assuming film flow. Solute transport in the macropores is described by a piston flow approach neglecting dispersion. Because the transport process in the macropore system is fast, it is assumed that sorption as well as degradation is negligible. Solute concentration at the upper boundary is calculated to be in equilibrium with the liquid concentration of the upper numerical layer of the soil matrix.

Initial water content for both runs (Plot 6) used the values given in Armstrong (1995) for 21 December 1990. During calibration, only the hydraulic parameters were changed in SIMULAT to optimise the simulated ground water level and drain flow. The pesticide sorption and degradation parameters were not modified, in accordance with the procedure suggested by Vanclooster et al. (2000).

Pesticide transport in the matrix is modelled in SIMULAT using the convection–dispersion equation. For Brimstone Farm, linear sorption in equilibrium with a single binding site was used. Linear sorption parameters ($K_d$) were taken from Harris et al. (1994), who measured 2.9 l/kg for isoproturon and 0.61 l/kg for mecoprop for this soil. In SIMULAT the degradation rate depends on water content and soil temperature. For Brimstone Farm, the degradation rate used an O’Neill function for temperature and an optimum curve for water content (Diekkrüger et al., 1995; Richter et al., 1996a, b), the overall rate being the product of these two functions. Estimates of the parameters were made from measurements of degradation rates at different soil temperatures and water contents given by Nicholls et al. (1993). For isoproturon, the half-life at 10°C and moisture content of 80% of Field Capacity was 200 days in the subsoil and 60 days in the topsoil (Harris et al., 1994).

The major problem with the SIMULAT representation of the Brimstone Farm site is that the water flowing through the macropores becomes drain flow only after passing through the soil matrix. The drainage water thus represents the water flowing through the soil matrix, not direct macropore flow as modelled by CRACK-NP and MACRO.

Table 5
Hydraulic parameters of Van Genuchten/Mualem and macropore model as used by SIMULAT. (Details of the parameters are given by Diekkrüger et al., 1995 and this issue)

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>Soil matrix</th>
<th>Macropore</th>
<th>Volume (cm³/cm³)</th>
<th>Lateral conductancea (mm/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\theta_s$ (cm³/cm³)</td>
<td>$\theta_r$ (cm³/cm³)</td>
<td>$\alpha$ (1/h Pa)</td>
<td>$N$</td>
</tr>
<tr>
<td>0–20</td>
<td>0.50</td>
<td>0.20</td>
<td>0.0006</td>
<td>1.9</td>
</tr>
<tr>
<td>20–40</td>
<td>0.53</td>
<td>0.20</td>
<td>0.0006</td>
<td>1.92</td>
</tr>
<tr>
<td>40–60</td>
<td>0.54</td>
<td>0.296</td>
<td>0.0204</td>
<td>1.26</td>
</tr>
<tr>
<td>60–200</td>
<td>0.49</td>
<td>0.227</td>
<td>0.0143</td>
<td>1.24</td>
</tr>
</tbody>
</table>

a Hydraulic conductivity divided by half the distance between the macropores.
2.4. PLM

PLM (Pesticide Leaching Model, version 3) is an empirical model, developed by Hall (1993); Hall and Webster (1993) and Nicholls and Hall (1995). Compared to the other models used in this exercise, it is a much simpler capacity-type model based on a daily water balance, in which water moves down the profile in ‘tipping-bucket’ fashion. Conceptually it is a development of the SL2 model (Addiscott, 1977) which subdivides the soil solution into mobile and immobile phases, with only the mobile water being displaced during drainage. PLM uses layers of 5 cm thickness and a calculation interval of one day. Because of this limitation, the model can only be used to simulate daily data, and so could not be used to model test data given at hourly intervals.

One layer can be specified to contain drains and a percentage of the water reaching that layer can pass into the drains, the remainder continuing to seep downwards. PLM does not simulate a water table and so the effects caused by a water table rising and falling is not modelled. The model uses daily weather data: rainfall, potential evapotranspiration, maximum and minimum air temperatures.

Sorption is simply estimated using linear \( K_d \) values. Sorption in the top layer increases gradually with time to simulate the slow diffusion of sorbate to sites less accessible to moving water. Degradation of herbicide is calculated as a function of temperature and soil-water content.

The broad dispersion and non-equilibrium sorption that occurs in macroporous soils is modelled by subdividing the mobile water into ‘slow’ and ‘fast’ categories. The percentage of ‘fast’ pores in the mobile phase needs careful calibration for each soil type. Data from Brimstone Farm had been modelled previously, and so, parameter values were used from previous modelling studies, and only adjusted where necessary. At Brimstone Farm, it is important to simulate the time and magnitude of the first drainage event, which carries the major pesticide load. The parameters in PLM that influence this are the initial soil–water deficit, the evaporation adjustment factor and the percentage of water removed by the drains. Initial calibrations were done by adjusting only the soil–water deficit. Concentrations of solute in drainage water are usually most sensitive to the macropore parameters. Initial calibrations are attempted by adjusting only the percentage ‘fast’ pores parameter.

The proportion of water entering the drains could not be predicted a priori using PLM. Calibration of the model was achieved by adjusting this value to 76% for Plot 9. The value adopted for Plot 6 was however 5%. These and the rest of the parameters used are given in Table 6.

Pesticide (isoproturon) parameters were derived from previous studies at the site. The sorption \( (K_d) \) parameters were 2.9 in the top 30 cm of the soil, 7.9 l/kg between 30 and 60 cm, and 2.0 l/kg below 60 cm. The half-life set at 208 days.

3. Results and discussion

The simulations are shown in a series of diagrams (Figs. 1–9) each having the same format and scale, so that the performance of each model can be compared directly. These
Table 6
Parameter values for the PLM model. (A description of the parameters is given by Hall, 1993)\(^a\)

<table>
<thead>
<tr>
<th>Depth cm</th>
<th>Total pore space (%)</th>
<th>Volumetric moisture content at 5 kPa</th>
<th>200 kPa</th>
<th>1500 kPa</th>
<th>Exclusion zone</th>
<th>Bulk density</th>
</tr>
</thead>
<tbody>
<tr>
<td>0–20</td>
<td>60.4</td>
<td>40.4</td>
<td>30.5</td>
<td>22.2</td>
<td>0.0</td>
<td>1.05</td>
</tr>
<tr>
<td>20–60</td>
<td>46.9</td>
<td>35.7</td>
<td>28.0</td>
<td>22.0</td>
<td>0.0</td>
<td>1.29</td>
</tr>
<tr>
<td>60–100</td>
<td>50.0</td>
<td>33.0</td>
<td>12.0</td>
<td>5.0</td>
<td>0.0</td>
<td>1.30</td>
</tr>
</tbody>
</table>

\(^a\) Depth to mole drains = 0.55 m; percentage water lost to drains = 5%; initial soil moisture deficit = 110 mm; drainage factor = 0.9; Hold back factor = 0.1; crop is none; evaporation reduction factor = 0.9; percentage of macropores = 80%; rate of ‘slow’ drainage = 60 cm/day; rate of ‘fast’ drainage = 120 cm/day.

MACRO (1)

Fig. 1. Calibrated model results using the MACRO model (User 1) for the short test period, 25 December 1990 to 14 January 1991. Modelled (dotted line) and observed (solid line) water table position; modelled (dotted line) and observed (*) isoproturon concentration in drainflow; modelled (dotted line) and observed (solid line) drain discharges.
Figures show the observed and predicted water table positions, plotted as depth below the surface, the observed and predicted concentrations of isoproturon in the drain waters, and the observed and the predicted discharges through the drainage system (Table 7). The relevant rainfall and PET data are shown in Harris et al. (2000).

The following discussions are based on the comparisons of hydrological behaviour (discharge and water table position) and the concentrations of isoproturon in the drainage

### Table 7

<table>
<thead>
<tr>
<th>Model</th>
<th>Observed Maximum Concentration (µg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observed</td>
<td>30.5</td>
</tr>
<tr>
<td>MACRO (User 1)</td>
<td>23.3</td>
</tr>
<tr>
<td>MACRO (User 2, uncalibrated)</td>
<td>486</td>
</tr>
<tr>
<td>MACRO (User 2, calibrated)</td>
<td>70.7</td>
</tr>
<tr>
<td>CRACK-NP</td>
<td>35.3</td>
</tr>
<tr>
<td>SIMULAT</td>
<td>0.659</td>
</tr>
<tr>
<td>PLM</td>
<td>149</td>
</tr>
</tbody>
</table>
water. Other aspects, for example the prediction of pesticide movement within the soil profile, are not presented here. Figs. 1–4 present the detailed simulations over the short test period (15 December to 15 January) during which detailed measurements of pesticide concentrations in the drainwater were available. Figs. 5–9 present the model results for long test period covering the whole of winter (October 1990 to March 1991). Because PLM only works on a daily time step, simulations were presented only for the longer period.

3.1. Short term test

3.1.1. MACRO-User 1

In general, the model simulates the observed behaviour over the short period relatively well. Here MACRO (Fig. 1) shows a remarkably good fit for all three components of the data. The model shows the build up of the water table, and the generation of the three drainage events in early January. These drainage events are accompanied by a peak of pesticide leaching.
The final predicted concentrations of isoproturon in the drainage water are all very similar to the observed, although they do fail to reproduce the height of the first peak. However, first runs of the model calibrated for the hydrology but using a larger mixing depth (1 mm) at the surface over-predicted the concentrations by an order of magnitude. It is thus clear that the MACRO model is very sensitive to this parameter, which controls the degree to which water flowing into macropores at the surface interacts with the solute in the matrix. Because of this adjustment to a critical parameter, these should be considered to be calibrated results from the model.

3.1.2. MACRO-User 2

The simulations from the second group, using the same model, (Fig. 2), are generally worse than those obtained by user 1, although when calibrated are close to those derived by user 1 using the same model. The model was initially evaluated and calibrated using

---

Fig. 4. Model results using the SIMULAT model for the short test period, 25 December 1990 to 14 January 1991. Modelled (dotted line) and observed (solid line) water table position; modelled (dotted line) and observed (*) measurements of isoproturon concentration in drainflow; modelled (dotted line) and observed (solid line) drain discharges.
the long-term set of data, and the best parameters for that longer dataset were then applied to the short test period without further calibration.

The initial uncalibrated run shows only a poor fit for the hydrology, with the water table rising later than observed, generating only a single peak of drainflow later than observed. The model predicts only a single pesticide-leaching event, which is over an order of magnitude greater than observed.

The calibrated runs show a better fit for the water table, and a generally good fit for the drainflow with the exception that it fails to predict the first drainflow event, and so misses the first pesticide leaching occasion. The subsequent calibrated run over-predicts the pesticide concentrations, giving a peak concentration of 70 μg/l which is roughly double that observed. In addition, the simulated leaching rate increases with time, not in agreement with the observed decrease.

The contrast between two sets of results using the same model (comparing Figs. 1 and 2) demonstrate the value of experience both with the use of the model and familiarity with the soil situation which resulted in better simulations by user 1.

3.1.3. CRACK-NP

CRACK-NP (Fig. 3) performed well, simulating the timing of the first discharge event, which is simultaneous with first rise of the water table above drain depth. The major
The success of the model is the accurate prediction of pesticide concentrations and the patterns of leaching. A major problem with implementing this, and indeed all the models, was the choice of the starting soil moisture conditions, and by varying these values slightly, the fit of the model could be improved. As fitted, the model over-predicted the second and third hydrographs, but modelled the leaching of isoproturon well. Part of this is a consequence of a limitation in the model in that it does not include a deep drainage routine, so that once the water table rises to drain depth it does not fall below it again. Consequently, the modelled soil is wetter than observed when presented with a second rainfall event, and the second hydrograph peak is thus larger than observed.

The pattern of isoproturon leaching differs from the leaching pattern for nitrate reported at the same site by Armstrong and Burt (1993). The pattern of isoproturon leaching shows a strong correlation with discharge, with each peak discharge event being followed by a rapid decline. This suggests that the mechanism that the model reproduces is closely tied to the pick up of solute held close to the surface of peds, which is then exhausted by the flows. This is in contrast with the pattern of nitrate leaching at the same site, in which the peaks of the discharge events are associated with a dip in concentration, suggesting that the process is limited by diffusion from within the aggregates (Armstrong and Burt, 1993).
SIMULAT (Fig. 4) gave a less successful simulation. When the water table rises to drain depth, this generates drain flow. This component, however, behaves too rapidly, so that the number of discharge peaks is too great and the water table falls too rapidly. This is a consequence of using the high value of 10 cm per day for the saturated hydraulic conductivity of the matrix.

The major problem with the results from SIMULAT is that pesticide concentrations are too low. This is because the drainage model was only linked to the matrix pore system. Therefore, all pesticides coming through the macropores have to infiltrate into the soil matrix before they could reach the drainage. Thus, the drainflow did not represent the macropore flow generated close to the soil surface.

3.2. Long-term test

The results of comparing the model predictions with the observations are shown in the same format (Figs. 5–9).

3.2.1. MACRO-User 1

MACRO (Fig. 5) simulated the pesticide concentrations for the longer period moderately well. The overall timing of the first discharge peak is predicted well, and the
good fit for the pesticide concentrations, already noted, is reproduced. The water table predicted by the model rises to drain depth, and then remain elevated. This reflects the lack of a slow drainage routine, which would reproduce the fall of the water table during the relatively dry period in January and February.

The major shortcoming of the dataset was the definition of the initial conditions, so most of the calibration effort concentrated on getting this initial state correct. The only other major correction was the reduction in the mixing depth, to zero, which reduced the degree to which water on the surface interacted with the pesticides retained in the topsoil. By reducing the value of this mixing length from 1 mm to 0, the concentrations of pesticide in the drainage waters were reduced by an order of magnitude, and the model then fitted the observations much more closely.

These results from MACRO illustrate the difficulty of getting the timing correct, which is partly a reflection of the way the meteorological data are reported. The rainfall reported in the meteorological files is, following the usual convention, the total rainfall in the previous 24 h reported at 9.00 a.m. on the day of recording. Models, however, normally take the rainfall in any day as relating to that day, and spread it over the 24 h period starting at midnight at the start of that day. MACRO in fact adopts a slightly different scheme, in that it distributes the rainfall at a constant intensity over as long a period as is necessary, starting at midnight, to give the right total. Because of this (or any other
arbitrary procedure that decomposes daily into hourly rainfall rates), the results of the model can appear to be temporally shifted by nearly one day compared to the observations. Clearly, the model reproduces the system behaviour quite well, but this time shift can produce a marked lack of fit, which is the consequence of the way the model handles the low time resolution input data. The reported results in Fig. 5 have thus been shifted one day to account for this mismatch.

3.2.2. MACRO-User 2

Starting with the soil parameters provided, the initial uncalibrated predictions of site hydrology produced by this group were poor. In this initial uncalibrated run (Fig. 6) the rise in the water table is too late, and so did not generate drainflow sufficiently early. Consequently, the initial peak of pesticide leaching was missed. The poor fit obtained with the first runs are a consequence of a lack of familiarity with the site, the model, and the limitations of the dataset. For example, the site data did not include any information on the distribution of moisture within the soil profile, either to provide an accurate starting point, or to act as a calibration check for the model performance.

The changes between the two runs were made exclusively in the hydraulic parameters (compare the two parts of Table 3), and attempted to remain as close as possible to the
original values. The major changes involved an increase in the hydraulic conductivity of the lower layers (thus speeding up the rise of the water table in the autumn), and increasing the water potential at which macropore flow is initiated. These two calibrations increased the degree of activity in the macropores and increased the vertical drainage.

The calibrated run predicted the rise in water table rather better, but then produced rather larger than observed amounts of drainflow. The uncalibrated run over-predicted the pesticide concentrations at the time of the first discharge peak, and then showed a continued decline thereafter. However, the calibrated results were close to the observed values, showing that it is possible to fit the model.

### 3.2.3. CRACK-NP

CRACK-NP predicts both the magnitude and timing of the major pesticide leaching event moderately well (Fig. 7). This is considered to be the result of the extensive development of the parameter set by other modelling studies at the same site, so that both the hydrological and pesticide behaviour parameters are based on firm data and past experience. Over the whole winter, the major shortcoming of the model is its failure to predict the fall and rise in water table between mid January and mid February between the two periods of rainfall. This is a consequence of the shortcoming of the model, already noted, that it lacks a slow drainage routine, so that the soil stays wetter between rainfall events than is actually the case. The consequence is that for the second period of rainfall, in March, CRACK-NP over-predicts the drainflow considerably. Work is currently underway to improve this component of the model.

### 3.2.4. SIMULAT

The simulations (Fig. 8) are similar to those observed for the shorter period. The model simulated the timing of the rise of the water table moderately well, but then simulated the first drainage event a little too early. The resulting drain flow thus appeared too early, and was too high. Because the Houghoudt drainage equation as implemented for the soil matrix is not a good representation of the performance of mole drainage, the predicted links between the water table and the drain flow later in the year are also only poorly modelled. However, the main deficiency of the model is in failing to simulate pesticide leaching at all well. The model simulated leaching of isoproturon at concentrations always less than 1, compared to the observed concentrations of up to 30 μg/l, because the macropores were not linked to the drainage model.

### 3.2.5. PLM

The PLM model was run for only a short period during the winter (Fig. 9). The drainage of water from the profile was under-predicted in January. PLM does not model the water table position. The isoproturon concentrations predicted by PLM are much larger than those observed. The maximum concentration predicted by PLM is 149 μg/l, compared with an observed value of 30 μg/l. PLM also simulated very rapid variation in concentrations from day to day during the runoff period, much greater than those observed at the site.
4. Conclusion

These results illustrate the difficulty of modelling the behaviour of water and pesticide movement in cracking clay soils. It is perhaps not surprising that the models developed with the explicit aim of representing macroporous soils, CRACK-NP and MACRO, performed rather better than the more generalised models, SIMULAT and PLM. Overall, the results of these comparisons imply that the best fits are those generated by the MACRO model as used by user 1, a combination of the most complete model and an expert user familiar with the conditions of the site, who nevertheless needed to perform some calibration. The same model produced less good (but still useful) results when used by the second group who were less familiar with the site. This clearly illustrates the absolute need for calibration of the model (whatever the model, the user and the site), especially where data on the hydrology of the site are limited. The CRACK-NP model also gave quite good results when used by modellers who were very familiar with the site. The results obtained by SIMULAT were poor, reflecting a failure in the model to represent the hydrological conditions of the site. PLM gave moderate results for the more limited task it addressed.

The use of the models also demonstrated the importance of soil–water measurements, particularly to define the initial conditions for the model runs. The lack of these data was a major shortcoming of the dataset distributed.

Acknowledgements

We thank our various colleagues for their help in the model runs, and our various funders, among the UK Ministry of Agriculture, Fisheries and Food, is gratefully acknowledged. The financial support for performing the comparison exercise was given by the COST 66 Action ‘Pesticides in the soil environment’ of DGXII-EU.

References

Aden, K., Diekkrüger, B., 2000. Modelling pesticide dynamics of four different sites using the model system SIMULAT. Agricultural Water Management.


