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Evaluation of uncalibrated preferential flow models against data for isoproturon movement to drains through a heavy clay soil

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Abstract: The uncalibrated predictive ability of four preferential flow models (CRACK-NP, MACRO/MACRO_DB, PLM, SWAT) has been evaluated against point rates of drainflow and associated concentrations of isoproturon from a highly structured and heterogeneous clay soil in the south of England. Data were available for four plots for a number of storm events in each of three successive growing seasons. The mechanistic models CRACK-NP and MACRO generally gave reasonable estimates of drainflow over the three seasons, but under-estimated concentrations of isoproturon over a prolonged period in the first season and over-estimated them in the two remaining seasons. CRACK-NP simulated maximum concentrations of isoproturon over the first two events of each of the three seasons of 156, 527 and 24.4 μg litre^{-1}, respectively, and matched the observed data (465, 65.1 and 0.65 μg litre^{-1}) slightly better than MACRO (69.1, 566 and 58.5 μg litre^{-1}). Automatic selection of parameters from soils information within MACRO_DB reduced the emphasis on preferential flow relative to the stand-alone version of MACRO. This gave a poor simulation of isoproturon breakthrough and simulated maximum concentrations were 0, 50.1 and 35.1 μg litre^{-1}, respectively. The capacity model PLM gave the best overall simulation of total drainflow for the first two events in each season, but over-estimated concentrations of isoproturon (967, 808 and 51.3 μg litre^{-1}). The simple model SWAT represented total drainflow reasonably well and gave the best simulation of maximum isoproturon concentrations (140, 80.2 and 8.2 μg litre^{-1}). There was no clear advantage here in using the mechanistic models rather than the simpler models. None of the models tested was able to simulate consistently the data set, and uncalibrated modelling cannot be recommended for such artificially drained heavy clay soils.

Keywords: drainflow; pesticide; cracking clay; regulatory; predictive; modelling

1 INTRODUCTION

Preferential flow refers to a situation where water infiltrating a soil does not equilibrate with the resident soil water, but flows rapidly to depth. For example, shrinkage cracks, earthworm channels or root holes may operate as flow pathways in which water moves rapidly downwards and by-passes the denser soil matrix.[1] In the sub-soil, permeable fill of drainage channels and mole drainage ruptures may also be of importance. Thereby, chemicals dissolved in the percolating water may move quickly out of the biologically and chemically reactive topsoil into the sub-soil where sorption is often weaker and degradation generally occurs at a lower rate. The risk of leaching of those chemicals to surface water and groundwater is thus greater.

The importance of preferential flow for the movement of pesticides has been demonstrated for a wide range of soils. Rapid movement to sub-surface drains appears to be a dominant pathway for pesticide transport to surface waters in heavy clay soils.[2,3] Pesticides by-passing the matrix of soils with intermediate texture may cause transient large concentrations moving to depth.[4,5] A description of preferential flow has been included in a number of mathematical models simulating pesticide transport through soil. The use of such models as a tool to support risk assessments within the pesticide regulatory process appears desirable. Currently, this is restricted by the lack of information on the predictive ability of preferential flow models and difficulties with the selection of input parameters.[6] The present study was initiated to give more information on this subject. The regulatory use of preferential flow models was evaluated using isoproturon concentrations in drainflow from a heavy clay soil in the south of England.

2 METHODS

2.1 The Brimstone Farm dataset

A long-term pesticide study has been carried out by

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ADAS and IACR-Rothamsted at Brimstone Farm, Oxfordshire, UK and has been described in detail elsewhere.[2,7,8] The site was established in 1978 and is located on a pelo-stagnogley of the Denchworth series. This soil type is characterised by a large clay fraction and a thick, slowly permeable subsoil. The main properties of the soil are summarised in Table 1. With an average annual rainfall of 686 mm, the climate is representative of many cereal-growing areas of central England.[9] The site comprised twenty hydrologically isolated 0.2-ha plots. The influence of selected unconventional management practices (eg generation of a fine tilth; application of a surface sealant) on pesticide losses was investigated on sixteen plots, whilst four plots received conventional treatment. Results from the four conventional plots were used for this study, as these were considered most representative of current agricultural practice. Two of the four control plots were conventionally mole-drained (plots 5 and 20). On one plot, the drainage system consisted of gravel-filled moles (plot 15), whilst the remaining plot had close-spaced pipes (plot 9). Data from three successive seasons were used for model evaluation. The herbicide isoproturon was applied to winter cereals on 2 November 1993, 17 November 1994 and 30 October 1995 at rates of 2.44, 2.50 and 0.25 kg ha^{-1}, respectively.

On each plot, surface runoff and drainflow were continuously monitored. Concentrations of isoproturon in drainage water were determined at frequent intervals. Sampling was carried out by automatic devices and triggered by flow. Residues of isoproturon in water were determined by reverse-phase high performance liquid chromatography with a diode-array detector. The limit of determination was 0.1 $\mu\text{g litre}^{-1}$. The identity of isoproturon in samples was confirmed by UV spectral analyses.

Detailed data on rates of drainflow for the three seasons and a number of point measurements of isoproturon concentrations were available, as well as total drainflow expressed by event and by season. Rainfall and maximum and minimum air temperatures were supplied at a daily resolution and potential evapotranspiration was estimated using Linacre's equation.[10] Further model input parameters were the isoproturon sorption coefficient K_d (2.9 ml g^{-1}) and the degradation half-life measured in the laboratory at 10 °C and 80% of field capacity (75 days) determined using soil from Brimstone Farm.[7]

2.2 Models

2.2.1 CRACK-NP

CRACK-NP is derived from the hydrological model CRACK,[11] which divides the total soil porosity into that within uniform aggregates and that in the cracks between. Water is assumed to move into aggregates according to Philip's infiltration theory[12] and out of them in response to crop extraction and/or evaporation. Downwards movement of water is assumed to occur only in the cracks, based on a theoretical analysis by Childs[13] with a modification to account for path tortuosity and connectivity. The assumption that there is no net flux of water within the soil matrix means that the model is only applicable for heavy clays where matrix flow can be considered to be a negligible component of total flow. Solute transport is modelled assuming mass flow in the cracks and diffusion, both within the aggregates and between cracks and aggregates. CRACK-NP version 2.0 was evaluated in this study. CRACK-NP was developed to describe data from earlier seasons at Brimstone Farm. Excellent fits to data from 1985/86, 1989/90 and 1990/91 using only measured parameters have been described.[14,15]

2.2.2 MACRO

MACRO[16] is a physically based preferential flow model with the total soil porosity divided into two flow domains (macropores and micropores). A separate flow rate and solute concentration is assigned to each domain. Water flow and solute transport in the micropores are modelled using Richards' equation[17] and the convection-dispersion equation, respectively. Fluxes in the macropores are based on a simpler capacitance-type approach with mass flow. Exchange between the two domains is calculated according to approximate, physically based expressions using an effective aggregate half-width. By varying the input parameters, the model can be set up to simulate a soil with nothing but preferential flow (as in CRACK-NP), a soil where preferential flow is insignificant, or any intermediate between these two extremes. This means that the model is appropriate to describe preferential flow in a variety of soils. Version 4.0 was used for this study.

MACRO has been evaluated in a number of recent field and lysimeter studies on leaching of pesticides and non-interactive solutes.[18–21] The results are generally promising, although marked discrepancies from measured data are occasionally observed. Calibrated simulations are often able to reproduce

Table 1. Selected characteristics of the Denchworth soil at Brimstone Farm

							Water content (cm^3 100 cm^{-3}) at kPa					
Depth (cm)	*C_{org} (%)*	*pH*	*Sand (%)*	*Silt (%)*	*Clay (%)*	*Bulk density (g cm^{-3})*	*0*	*−5*	*−10*	*−40*	*−200*	*−1500*
0–24	3.6	7.6	10.5	29.5	60.0	1.00	56.8	55.2	54.6	48.4	44.3	37.4
24–52	1.1	8.0	10.5	25.0	64.5	1.18	48.5	46.1	45.6	43.8	41.3	33.5
52–68	0.9	8.2	5.6	21.4	73.0	1.22	52.6	51.2	50.6	48.2	46.5	38.0

observed leaching of pesticides. Simulations without calibration are less frequently performed, due to continuing difficulties with selection of appropriate input parameters. Uncalibrated MACRO runs can, however, show an improved match to observed transport behaviour for a range of soils relative to models without preferential flow.[22]

2.2.3 MACRO_DB

MACRO_DB[23] is a version of the MACRO model which is linked to various data sources. The databases provided include pesticide properties, soils, cropping and weather. The system will automatically select input parameters from soil information using a combination of simple rules and 'pedo-transfer functions' and then run MACRO. MACRO_DB has been designed for the non-specialist user making exposure and risk assessments for pesticides. Given the complex nature of modelling preferential flow, it is likely that MACRO_DB will be used within pesticide risk assessments to parameterise and run the model for selected scenarios. It is thus important to evaluate the validity of the complete system (ie the MACRO model in combination with parameter selection routines). In this study, this was done by simulating the behaviour of isoproturon with MACRO on the basis of parameters automatically selected with MACRO_DB. Results were compared with those simulated with MACRO following parameter selection using experimental data and expert judgement. The version of MACRO_DB which is linked to MACRO 4.0 was used in this study. It should be noted that automatic parameter selection and subsequent simulations with the MACRO model are in the following text referred to as simulations with MACRO_DB.

MACRO_DB has been released for approximately 4 years. At present, no evaluations of the parameter estimation routines have been reported in the literature.

2.2.4 PLM

The Pesticide Leaching Model (PLM)[24] is a semi-empirical capacity model which divides the soil profile into 5-cm layers and the soil water into mobile and immobile phases. The mobile water is defined as the water content at tensions between field capacity ($-5\,\text{kPa}$) and saturation. This phase is further divided into a 'slow' and a 'fast' flow domain to account for both convective flow of soil solution through the soil matrix and rapid preferential flow through macropores or fissures. The empirical parameters which define the percentage of the mobile phase characterised as 'fast' and the depth leached per time interval in the fast and slow regions need to be specified by the user, based on expert judgement.

PLM has been successfully calibrated to simulate transport of bromide and chloride through lysimeters with two different soil types.[25] Calibration of PLM to describe dichlorprop leaching through lysimeters with three Swedish soils was also possible although, in common with other models tested, it was necessary to increase the half-life in soil by up to an order of magnitude relative to that measured in the laboratory.[26]

2.2.5 SWAT

SWAT is a semi-empirical model which has been developed to predict concentrations of pesticides moving to surface waters via the combined pathways of overland flow, lateral sub-surface flow and drainflow.[27] It assumes a direct hydrological link between soil type and the amount of water moving rapidly to streams in response to rainfall, which has been reported as the Hydrology of Soil Types (HOST).[28] This system groups all UK soil series into twenty-nine classes based upon hydrological characteristics of the soil and the underlying substrate layer. Using the HOST system, soils have been grouped according to their potential for run-off into five classes. These classes form the basis for prediction of the movement of water and associated pesticide to streams in response to rainfall. Partition and 'attenuation factors' account for pesticide sorption and the decrease in concentrations between events, respectively.

SWAT has been evaluated against data from three field studies on a range of soils with a number of contrasting pesticides.[27] The model was shown to be capable of predicting to within one order of magnitude the transient peak concentrations of a wide range of pesticides during rapid water movement to streams in response to rainfall. Simulated concentrations were too large when rainfall initiated water movement to streams very soon after application, particularly for the more mobile pesticides. Predictions for pesticides sorbed very strongly to soil were relatively poor.

2.3 Approach to model evaluation and parameter selection

For regulatory purposes, modelling is often used to evaluate environmental processes, with detailed field work only triggered if adverse simulation results are obtained. Thus preferential flow models will often be used in a purely predictive capacity with no experimental data available against which to calibrate input parameters. Accordingly, calibration was avoided in this evaluation study wherever possible, and input parameters for modelling were selected from basic information (measured soil properties and water release curves, soil profile description, measured degradation and sorption properties, site-specific information on the drainage system and crop growth). An exception was initial soil moisture conditions for PLM (Section 2.3.4). Soil profile depth was set to below drain depth for all models. This improves the numerical stability of the simulations and does not affect simulated drainflow or pesticide concentrations. Simulated volumes of drainflow and maximum concentrations of isoproturon for each of the events were compared with the observed data.

2.3.1 CRACK-NP

CRACK-NP simulations with version 2.0 of the model were based on an input file for Brimstone Farm which was provided by the model developers for the 1990/91 season for modelling with version 1.0. The parameters for this input file were derived from measured data as far as possible.[14] Measurements were available for soil hydraulic properties, crack spacing, ped sorptivity and stable drainable porosity. In our study, application rates and dates, cropping dates and pesticide properties were changed to match those specific to the years considered. The simulations were started 11–50 days before the first leaching event (2 November 1993, 7 November 1994 and 30 October 1995). An earlier start was not possible, because this destabilised the model. As no measured data were available, initial water contents were set to field capacity at the start of the simulation. The main soil physical and hydraulic input parameters for CRACK-NP to simulate the movement of water and isoproturon during 1993–1996 are given in Appendix 1. It should be noted that some of the parameters used for CRACK-NP (for example bulk density, field capacity) differ from those used for the other models (see Appendices 2–4). Initially, attempts were made to adapt the input file for CRACK-NP, but this resulted in model instability. It was thus decided to use the file provided by the model developers for the 1990/91 season with only minor changes.

Two of the parameters influencing crop evaporation for CRACK-NP are the crop interception capacity for rainfall and the factor to correct evapotranspiration from a wet canopy relative to potential evapotranspiration. These were set to 5 mm and 1.5, respectively, in the input file provided with the model. Attempts were made to adjust these values to those used for MACRO (2 mm and 1.0, respectively), because the latter values were considered more realistic. This destabilised the model which then crashed. In initial model runs, actual simulated evapotranspiration was considerably larger than potential evapotranspiration. This suggested that there are weaknesses in the model subroutine calculating actual evapotranspiration. In order to evaluate the description of preferential flow used in CRACK-NP independent of these weaknesses, an unrealistic compensation was made and the model was run assuming that the soil was bare over the 1993/94 and 1994/95 seasons.

2.3.2 MACRO

Input parameters for MACRO were derived from measured data as far as possible to limit user-subjectivity. An exception was the parameter describing the relative proportion of sorption sites in the macropore region (FRACMAC) which was set to 0.01 (1% of sorption sites are in the macropores). This was considered more realistic than the default value (0.1) used in MACRO version 4.0 (N Jarvis, pers comm).

Expert judgement was used to establish the parameter value for water tension at the boundary between the two flow domains (CTEN) as this cannot readily be estimated independently. A value of -5 kPa was selected for the heavy clay soil at Brimstone Farm. The water content equivalent to this tension (XMPOR) and the pore-size distribution index in the micropores (ZLAMB) were derived from measured water-release data whilst the conductivity at the boundary (KSM) was estimated using the equation given by Laliberte *et al.*[29] The pore-size distribution index in the macropores (ZN) was calculated from CTEN using equations built into MACRO_DB.[23] Saturated conductivity (KSATMIN) was derived using a pedo-transfer function for clay and loam soils in England and Wales (eqn (1)).[30]

$$\mathrm{KSATMIN} = 18.13 - 4.62\mathrm{AC} + 0.538\mathrm{AC}^2 \qquad (1)$$

where KSATMIN = saturated hydraulic conductivity ($\mathrm{mm\ h^{-1}}$)

AC (air capacity) =
total porosity − water content at − 5kPa (% vol)

The parameter aggregate half-width (ASCALE) controls the movement of water and solute between the micropore and macropore domains. Values were selected from basic descriptions of soil structure using the rules proposed by Jarvis *et al.*[23] The model was run for at least 3 months before any of the measured drainflow events. In the absence of measured values, initial soil water content was set to establish drainage equilibrium (ie fully wetted but without initiating drainflow). The main soil physical and hydraulic input parameters for MACRO are given in Appendix 2.

2.3.3 MACRO_DB

The weather, pesticide, application and site hydrology (drain depth, drain spacing, depth of profile) parameters used within MACRO were retained. These input values were combined with a set of crop parameters selected from the database provided with MACRO_DB (winter wheat at a German location). The dates of emergence and harvest were altered to match those at Brimstone Farm. Soil hydraulic parameters were calculated within MACRO_DB from soil analyses (soil organic carbon content, texture and bulk density given in Table 1).[23] The main parameters for MACRO_DB are compared with those for MACRO in Appendix 2. The parameter describing the relative proportion of sorption sites in the macropore region (FRACMAC) is also set within the system according to soil properties[23] and was 0.04 for the Denchworth soil at Brimstone Farm.

2.3.4 PLM

The main soil physical and hydraulic input parameters for PLM are given in Appendix 3. The percentage of mobile water prone to fast flow within PLM is difficult to derive from soil properties, but values close to 100% were considered reasonable for heavy clay soils where preferential flow is the dominant pathway for water

Table 2. Comparison between total flow (mm) observed in the six events at Brimstone Farm and those simulated in uncalibrated runs with the preferential flow models

Season	*Event*	*Observed*[a]	*CRACK-NP*	*MACRO*	*MACRO_DB*	*PLM*	*SWAT*
1993/94	13–15 Nov 93	5.1 (±1.2)	0.5	3.6	1.9	3.8	5.3[b]
	8–9 Dec 93	10.4 (±2.2)	1.7	2.1	0.6	8.7[b]	6.3
1994/95	8–9 Dec 94	8.3 (±5.0)	11.6[b]	10.0[b]	5.9[b]	3.5[b]	9.8[b]
	28–29 Dec 94	17.9 (±8.6)	13.5[b]	15.1[b]	11.7[b]	24.4[b]	16.4[b]
1995/96	19–23 Dec 95	51.5 (±8.6)	52.2[b]	56.9[b]	47.6[b]	44.3[b]	33.0
	6–10 Jan 96	6.8 (±4.7)	0.8	5.4[b]	1.1	10.8[b]	6.4[b]

[a] Mean of values for plots 5, 9, 15 and 20 together with SD in parentheses.

[b] Simulated value within mean ± SD of observed.

movement. A value of 95% was chosen for modelling the Brimstone Farm dataset. The slow and fast flow rate were set to 5 cm day^{-1} and 70 cm day^{-1}, respectively. Initial soil moisture deficits for the three seasons (ie the amounts of water required to increase soil moisture to field capacity) were calibrated such that the simulated and observed drainflow started approximately on the same date. This was necessary as PLM does not enable the user to simulate an initiation period before pesticide application. It should be noted that a calibration of initial water contents is usually not possible for regulatory risk assessments. However, these assessments often focus on the overall behaviour of a pesticide (average losses or concentrations). In contrast, this study compared the simulated and observed timing of breakthrough and patterns of leaching. The calibration of initial water contents was considered necessary to ensure a valid comparison with the remaining models. PLM simulates drainage by partitioning the water leaching from the bottom of the soil profile into that intercepted by the drains and that lost via seepage. All water was assumed to be intercepted by the drains in this study.

2.3.5 SWAT

SWAT only requires basic soil information to run, and input parameters were taken from measured data, apart from hydraulic conductivity at field capacity, which was derived as described by Brown and Hollis.[27] The input parameters for SWAT are listed in Appendix 4.

3 RESULTS AND DISCUSSION

3.1 Simulation of drainflow

The preferential flow models were used to simulate drainflow over the three seasons at Brimstone Farm. Table 2 summarises simulated drainflow totals for the first two events in each of the three seasons. Comparing the simulated flow with the mean ±1 SD shows that the mechanistic models CRACK-NP and MACRO_DB were accurate for three of the six events, MACRO for four events. SWAT and PLM have relatively simple hydrological routines, but flow totals were within the mean ±1 SD of that observed for four and five of the six events, respectively.

Figure 1 shows the patterns of flow simulated by

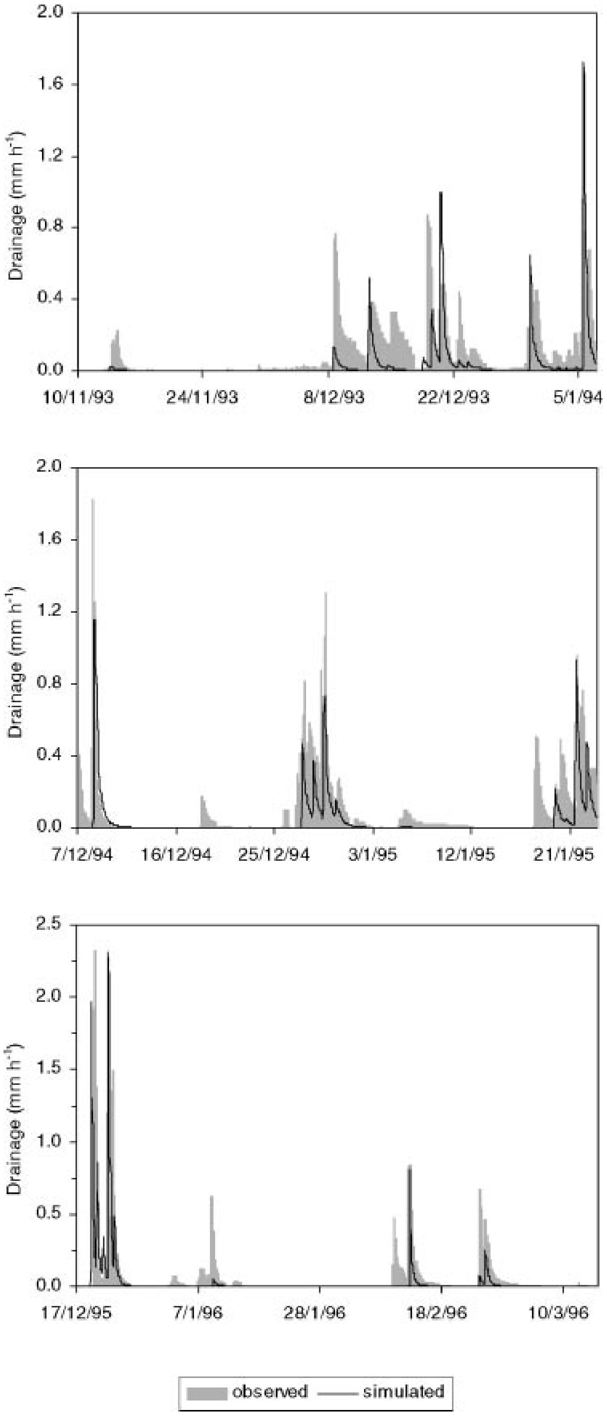

Figure 1. Comparison between observed rates of drainflow from plot 9 at Brimstone Farm and those simulated by CRACK-NP.

CRACK-NP in comparison with observed data from one of the four plots (plot 9) for each of the three seasons. In 1993/94, flow was under-estimated by the model, although the timing of events was relatively closely matched. Simulated hydrographs for the second season were similar to those observed, but the onset of drainflow often occurred too late. CRACK-NP performed relatively well for the first event of the 1995/96 season, but under-estimated drainflow later in the season (Fig 1). It should be noted that CRACK-NP was run assuming that the soil was bare over the 1993/94 and 1994/95 seasons.

Results of MACRO simulations were very similar to those from CRACK-NP, although MACRO simulated larger peak rates of flow. In contrast, the input parameters selected using the automatic procedures within MACRO_DB significantly under-estimated the importance of preferential flow. Smoother hydrographs and less total drainflow were simulated (Fig 2). Flow for several events was significantly under-estimated and it is concluded that simulations using parameters derived from first principles are more representative of hydrology at the site than those derived using the automated procedures within MACRO_DB.

More detailed analysis of hydrological simulations by PLM and SWAT is not appropriate for the current dataset, because model output is on a daily resolution or for whole events, respectively.

3.2 Simulation of isoproturon leaching

There was considerable variability in concentrations of isoproturon in drainflow from the four plots (Fig 3). Mean and standard deviation of maximum isoproturon concentrations in drainflow for the first two events in each season are presented for the four plots in Table 3 and compared with those simulated by the various models. Experimental data show that the first events of the season are disproportionately important for total losses of pesticide in drainflow from Brimstone Farm.[8]

Of the 30 maximum concentrations simulated, only one (CRACK-NP for the second event in 1993/94) falls within 1 SD of the mean observed. This clearly demonstrates the difficulty of simulating this site without comprehensive calibration. Taking a broader measure of acceptability of within one order of magnitude of the observed mean, CRACK-NP, MACRO and SWAT were acceptable for both events in 1993/94 and the first event in 1994/95. For the same three events, PLM was acceptable for two events and MACRO_DB for one. None of the models gave acceptable simulations for the second event in 1994/95 or either event in 1995/96.

Comparison of the maximum concentration of isoproturon observed and simulated over the first two events of each season (Table 3) shows that PLM over-estimated concentrations by a considerable margin in all three seasons, whilst CRACK-NP, MACRO and SWAT under-estimated concentrations in the first season and over-estimated them in the two subsequent seasons. SWAT and PLM were the only models to simulate correctly the relative magnitude of maximum concentrations in each of the three seasons (ie 1993/94 > 1994/95 > 1995/96), and SWAT gave the best overall simulation of maximum concentrations for the six events. A dominant factor used by SWAT to estimate concentrations moving to surface waters is the time from application to the storm event. As this was shortest in 1993/94, the largest concentrations were simulated in this year. CRACK-NP and MACRO

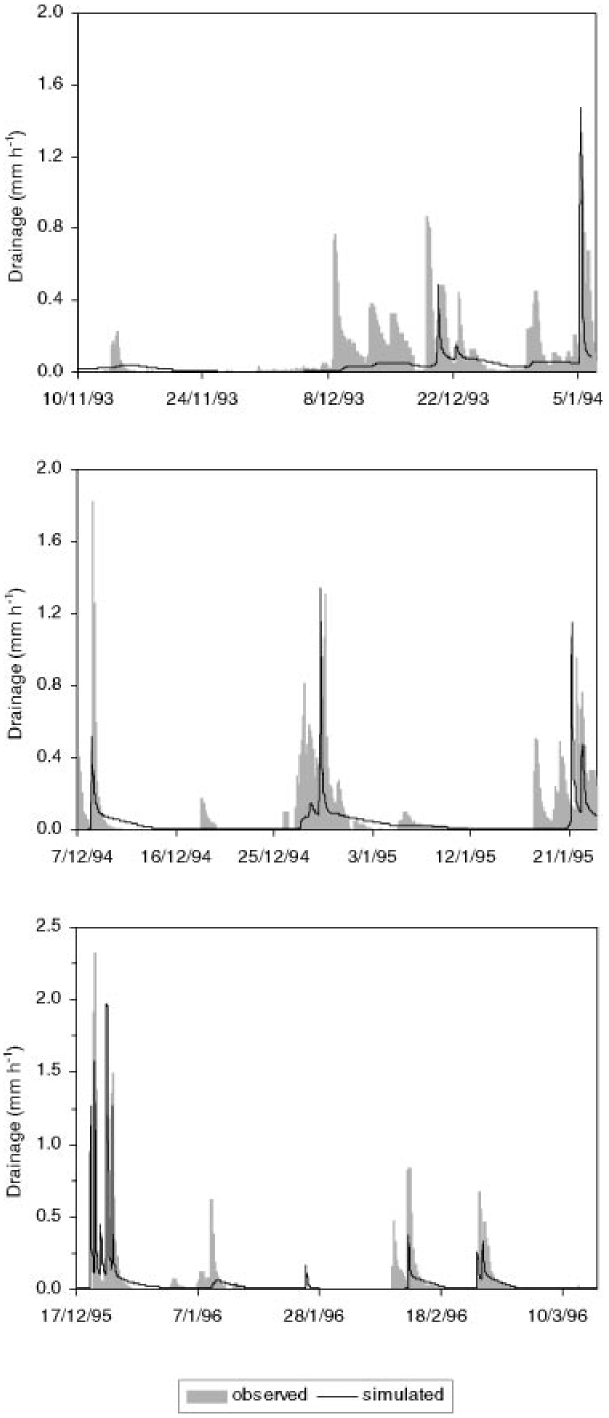

Figure 2. Comparison between observed rates of drainflow from plot 9 at Brimstone Farm and those simulated by MACRO_DB.

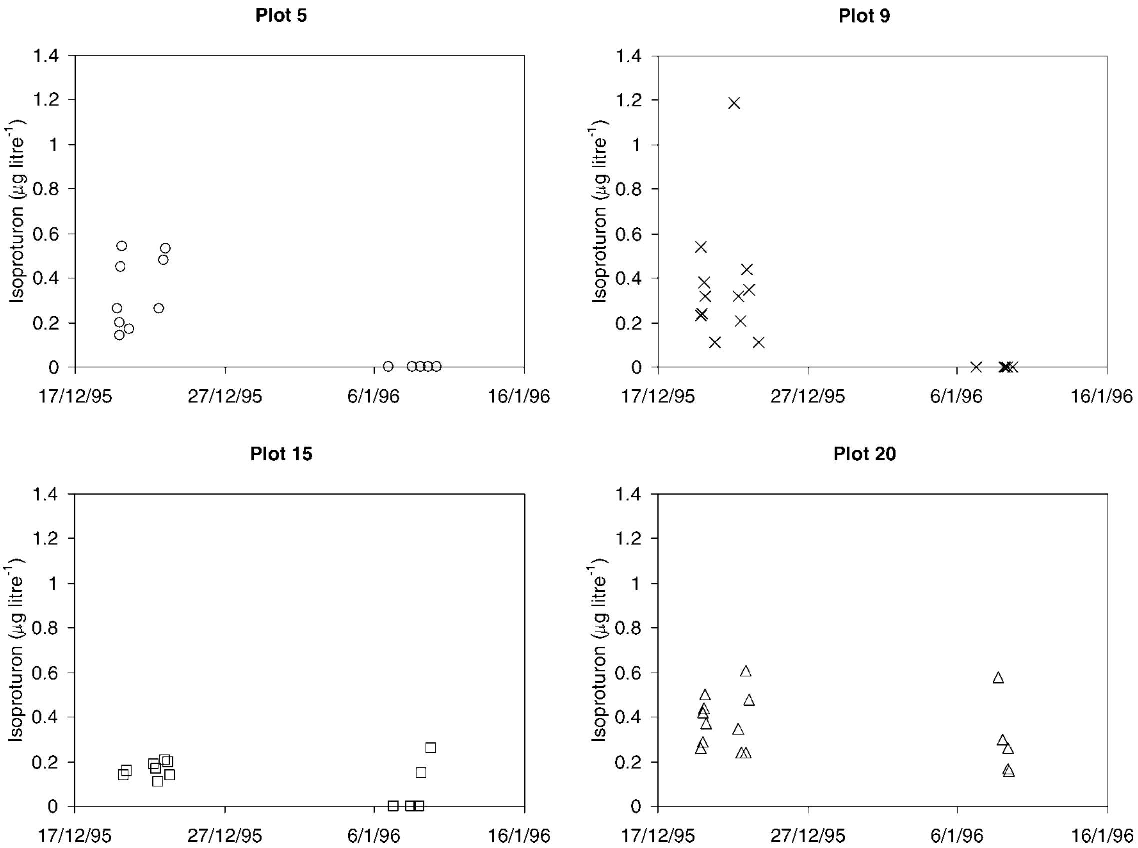

Figure 3. Concentrations of isoproturon observed in two events in drainflow from four plots at Brimstone Farm (1995/96).

include additional effects which resulted in much larger concentrations being simulated for the second season than for the first. Time from application to the first drainage event has been shown to be critical in determining losses of pesticides to drains at Brimstone Farm.[31]

Figure 4 shows observed concentrations of isoproturon in drainflow and those simulated by CRACK-NP. For clarity, only the results for plot 9 are presented. CRACK-NP matched the pattern of concentrations in drainflow in 1993/94 relatively well, even though the simulation of hydrology was poor over this period (Figs 1 and 4). In the second and third seasons, for which drainflow was better simulated by CRACK-NP, isoproturon concentrations were markedly over-estimated by the model.

The isoproturon concentrations in drainflow simulated by MACRO are compared with observed data for plot 9 in Fig 5. Concentrations were poorly simulated. Results for the 1993/94 season were best, but the model under-estimated peak concentrations for the first and second events and over-estimated them later in the season. In both subsequent seasons, peak concentrations were greatly over-estimated by MACRO.

The range of maximum concentrations observed over the three seasons spans two orders of magnitude if normalised to a single application rate. Neither CRACK-NP nor MACRO was able to mimic these relative differences. In part, this is accounted for by the absence of information on initial water contents and rainfall intensity. Nevertheless it appears that some of the processes determining pesticide transport at Brimstone Farm were not adequately described by the two models. Alternatively, the measurements taken at the site may be insufficient to characterise the processes and thus fully parameterise the models.

Table 3. Comparison between maximum concentrations of isoproturon (µg litre^{-1}) observed in the six events at Brimstone Farm and those simulated in uncalibrated runs with the preferential flow models

Season	*Event*	*Observed*[a]	*CRACK-NP*	*MACRO*	*MACRO_DB*	*PLM*	*SWAT*
1993/94	13–15 Nov 93	465 (±132)	156	69.1	0	967	140
	8–9 Dec 93	134 (±47)	141[b]	55.7	0	682	43.4
1994/95	8–9 Dec 94	65.1 (±14.7)	527	566	8.2	808	80.2
	28–29 Dec 94	2.6 (±2.3)	206	524	50.1	613	37.3
1995/96	19–23 Dec 95	0.65 (±0.39)	24.4	58.5	35.1	51.3	8.2
	6–10 Jan 96	0.21 (±0.28)	5.3	12.4	2.9	35.4	3.9

[a] Mean of values for plots 5, 9, 15 and 20 together with SD in parentheses.

[b] Simulated value within mean ± SD of observed.

For example, detailed information on soil structure was not available, but aggregate size has been shown to have a significant effect on both actual and simulated pesticide leaching.[19]

Automatic parameter selection using the routines built into MACRO_DB reduced the influence of preferential flow compared with the stand-alone version of MACRO. The consequence of this difference was smaller isoproturon concentrations in drainflow. MACRO_DB failed to predict any concentrations of isoproturon at all in drainflow early in the 1993/94 season when the largest concentrations occurred, and the pattern of concentrations in all seasons was poorly matched (Table 3). Coupled with the overall weaker simulation of water flow, this shows that simulations with MACRO_DB are poor for this soil type.

Again, more detailed analysis of output from PLM and SWAT is not appropriate because of the time-step for output from the models.

3.3 Overall assessment

Water and solute movement observed at Brimstone

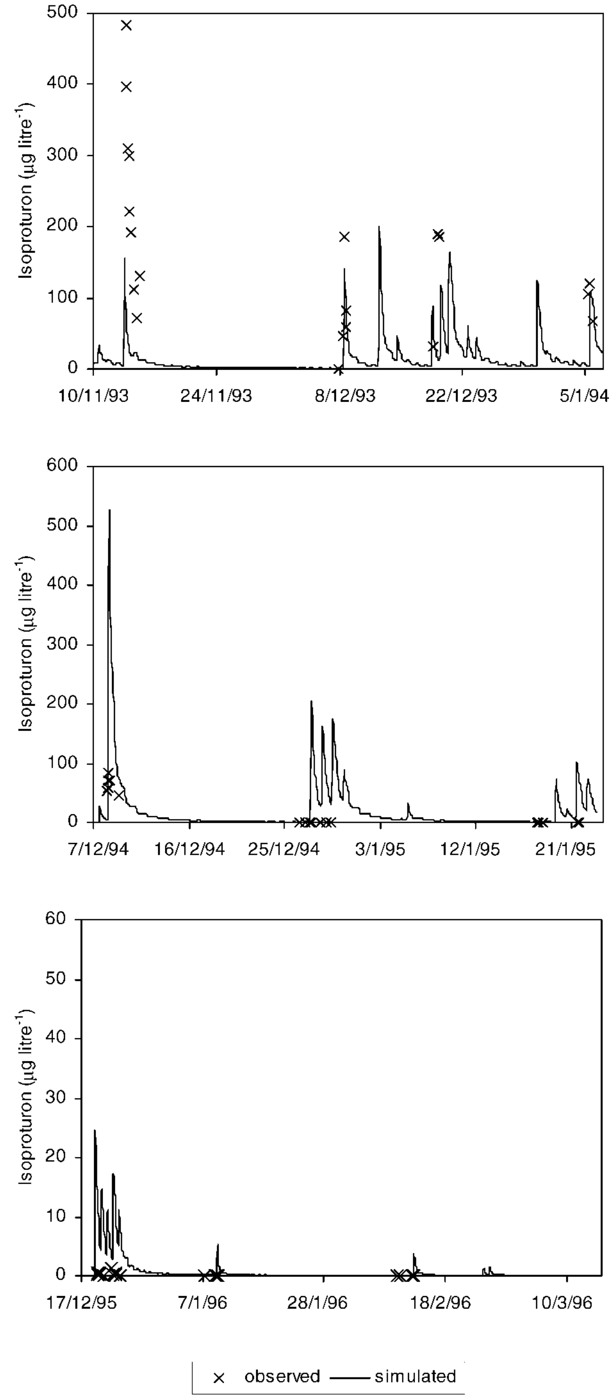

Figure 4. Comparison between observed concentrations of isoproturon in drainflow from plot 9 at Brimstone Farm and those simulated by CRACK-NP.

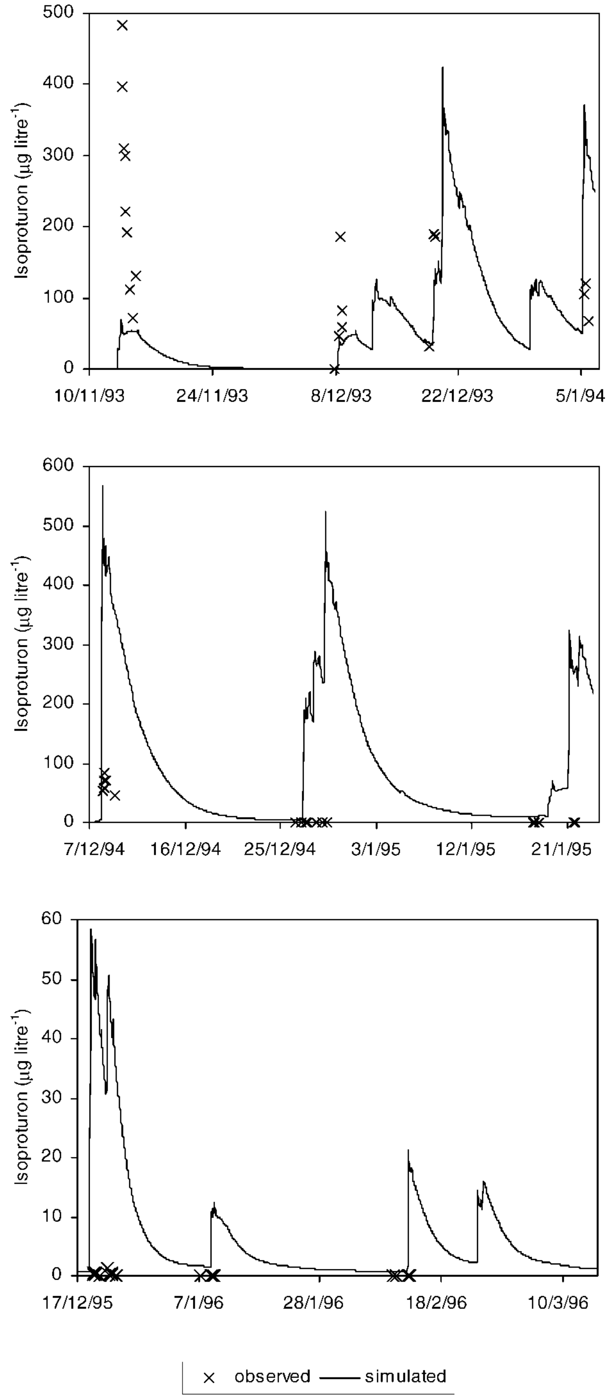

Figure 5. Comparison between observed concentrations of isoproturon in drainflow from plot 9 at Brimstone Farm and those simulated by MACRO.

Farm in previous seasons were described successfully with CRACK-NP.[14,15] It was, therefore, expected that the experimental data from 1993–1996 at Brimstone Farm might be relatively well simulated by the model. However, the spatial and temporal variability in water and pesticide leaching at the site made an extrapolation difficult. With regard to drainflow, the mechanistic models CRACK-NP and MACRO performed in a similar way, and neither clearly out-performed the other. Pesticide movement at Brimstone Farm was simulated somewhat better by CRACK-NP than by MACRO, but there were still large discrepancies with observed concentrations in two of the three seasons.

A drawback of both CRACK-NP and MACRO is their complexity, which leads to uncertainties in parameterisation. In particular, sensitive parameters describing macroporosity are difficult to select. MACRO_DB aims to reduce these difficulties by using automatic parameter estimation routines. However, the system under-estimated the importance of preferential flow in two of the three seasons simulated here, suggesting that the parameter estimation methods need to be improved for this soil type. The system has not been independently validated and significant testing against field data is required.

Two relatively simple models, PLM and SWAT, were included in the evaluation. PLM was the only model for which a genuine calibration of initial water contents was carried out (because of a limitation preventing a pre-run to bring hydrological conditions to equilibrium prior to pesticide application). PLM gave the best overall simulation of total volumes of drainflow over two events of each season, but markedly over-estimated isoproturon concentrations in all three seasons. SWAT gave the best overall simulation of maximum concentrations of isoproturon in drainflow. The model aims to aggregate the spatial and temporal variability associated with preferential flow up to field scale. PLM and SWAT both work on a relatively coarse temporal resolution. However, when expressing results on the basis of whole events, there was no clear advantage in using the mechanistic models rather than the simpler models in the current exercise. It appears that a number of processes are insufficiently characterised at present to allow a fully mechanistic description of the complex behaviour of pesticides in heavy clay soils.

3.4 Implications for regulatory modelling

None of the four preferential flow models consistently simulated the data on drainflow and pesticide losses at Brimstone Farm within acceptable levels of accuracy. Results suggest that simulation of such a heavy clay soil with artificial drainage systems without calibration carries a high risk of inaccuracy. The use of the models tested for regulatory assessments of pesticide leaching through heavy clay soils should not be recommended without calibration.

The parameterisation of preferential flow models is difficult. Additional measurements (eg hydraulic conductivity of the soil matrix, soil water contents at near saturation) can improve this situation. Sensitivity analysis specific to the model and scenario to be simulated is required to guide additional experimentation and the evaluation of model output.

The failure of the models to consistently describe the dataset can partly be attributed to the extreme variability of pesticide concentrations at Brimstone Farm between seasons and plots. The variability between the four plots was in part due to the fact that they were not true replicates in terms of drainage treatments. In addition, the spatial variability of soil properties influencing preferential flow (for example crack spacing and stability) and their temporal variation due to management practices and weather conditions leads to an extreme variability of results obtained at different points and times within the same field. This implies that it is misleading to carry out a deterministic simulation of pesticide behaviour in such soils. Rather, stochastic treatments should be used which incorporate the variability to predict a range of possible pesticide concentrations. Probabilistic approaches are appropriate only where the model shows a reasonable potential to simulate the processes governing pesticide transport and this does not seem to be the case for this soil type. Further research is required into the processes controlling pesticide transport in soils prone to extreme preferential flow and this should eventually feed into improved mathematical models.

Although the preferential flow models evaluated in this study were not able to simulate movement of a pesticide through this heavy clay soil, they have been demonstrated to perform better for a range of intermediate soils.[22] For such soil types, preferential flow models appear to be able to simulate pesticide leaching with a degree of accuracy and have clear advantages in representing reality over models which do not take this process into account.

4 CONCLUSIONS

None of the preferential flow models tested in this study consistently simulated water and isoproturon movement through the highly-structured heavy clay soil at Brimstone Farm in an adequate way. This can be attributed to the large spatial and temporal variability of factors influencing water and isoproturon movement at the site and the failure of the models to treat accurately all relevant controlling processes. When expressing results on the basis of whole events, there was no clear advantage here in using the mechanistic models rather than the simpler models. The use of the models tested for regulatory assessments of pesticide leaching through heavy clay soils should not be recommended without calibration. However, the findings of this study do not extend to the potential for the models to more accurately simulate water and pesticide movement through other soil types.

APPENDIX 1
Soil physical and hydraulic input parameters for CRACK-NP

Parameter	*Soil depth (cm)*	*CRACK-NP*
Crack spacing (m)	0–5	0.05
	10–20	0.08
	20–40	0.2
	40–60	0.3
	60–100	0.4
Tortuosity (–)	0–100	2
Ped sorptivity (mm h$^{-0.5}$)	0–100	12
Shrinkage characteristic (–)	0–20	0.0
	20–40	0.5
	40–60	0.8
	60–100	1.0
Bulk density topsoil (g cm^{-3})	0–20	1.12
Bulk density subsoil (g cm^{-3})	20–100	1.40
Hydraulic conductivity (mm h^{-1})	0–100	20
Total porosity (cm^3 100 cm^{-3})	0–60	55
	60–100	50
Field capacity (cm^3 100 cm^{-3})	0–20	48
	20–40	52
	40–60	50
	60–100	46
Stable drainable porosity (cm^3 100 cm^{-3})	0–20	5
	20–40	2
	40–60	1
Wilting point (cm^3 100 cm^{-3})	0–20	27
	20–60	35
	60–100	30

APPENDIX 2
Soil physical and hydraulic input parameters for MACRO and MACRO_DB

Parameter	*Soil depth (cm)*	*MACRO*	*MACRO_DB*
Aggregate half-width (mm)	0–16[a]	40	40
	16–24[a]	100	100
	24–52	30	30
	52–60	75	75
Bulk density (g cm^{-3})	0–24	1.00	1.00
	24–52	1.18	1.18
	52–60	1.21	1.22
Hydraulic conductivity (mm h^{-1})	0–24	12.1	100
	24–52	10.1	81.5
	52–60	12.7	1.61
Boundary hydraulic conductivity (mm h^{-1})	0–24	0.0135	0.0960
	24–52	0.0084	0.0580
	52–60	0.0109	0.0280
Boundary tension (cm)	0–24	50	20
	24–52	50	23
	52–60	50	32
Boundary water content (cm^3 100 cm^{-3})	0–24	55.2	58.1
	24–52	46.1	51.5
	52–60	51.2	51.2
Total porosity (cm^3 100 cm^{-3})	0–24	56.8	62.1
	24–52	48.5	56.0
	52–60	52.6	54.6
Wilting point (cm^3 100 cm^{-3})	0–24	37.4	35.4
	24–52	33.5	33.3
	52–60	38.0	34.8
Residual water content (cm^3 100 cm^{-3})	0–60	0	0
Pore size distribution of micropores (–)	0–24	0.069	0.075
	24–52	0.051	0.067
	52–60	0.060	0.063
Pore size distribution of macropores (–)	0–60	5.8	5.0

[a] The boundary between the upper two soil layers was set to 18-cm depth for MACRO_DB.

APPENDIX 3
Soil physical and hydraulic input parameters for PLM

Parameter	*Soil depth (cm)*	*PLM*
Bulk density (g cm^{-3})	0–25	1.00
	25–50	1.18
	50–70	1.22
Drainage coefficient (α) (–)	0–70	0.9
Hold-back factor (β) (–)	0–70	0.1
Proportion of fast mobile phase (%)	0–70	95
Rate of slow drainage (cm day^{-1})	0–70	5
Rate of fast drainage (cm day^{-1})	0–70	70
Total pore space (cm^3 100 cm^{-3})	0–25	56.8
	25–50	48.5
	50–70	52.6
Water at −5 kPa (cm^3 100 cm^{-3})	0–25	55.2
	25–50	46.1
	50–70	51.2
Water at −200 kPa (cm^3 100 cm^{-3})	0–25	44.3
	25–50	41.3
	50–70	46.5
Water at −1500 kPa (cm^3 100 cm^{-3})	0–25	37.4
	25–50	33.5
	50–70	38.0

APPENDIX 4
Soil physical and hydraulic input parameters for SWAT

Parameter	*SWAT*
Soil runoff potential class	S1
Bulk density (g cm^{-3})	1.00
Hydraulic conductivity at −5 kPa (mm day^{-1})	2.27
Total pore space (cm^3 cm^{-3})	0.568
Water at −5 kPa (cm^3 cm^{-3})	0.552
Water at −40 kPa (cm^3 cm^{-3})	0.484
Water at −200 kPa (cm^3 cm^{-3})	0.443
Water at −1500 kPa (cm^3 cm^{-3})	0.374

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