Development of guidance on parameter estimation for the preferential flow model MACRO 4.2

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The opinions expressed and conclusions drawn in this report are those of the authors and not necessarily of the project’s sponsor.

COMMENTS FROM THE MODEL DEVELOPER

A draft of this report was sent to the developer of MACRO, Prof. Nick Jarvis, Swedish University of Agricultural Sciences for comment. A number of comments for clarification, changes in emphasis and interpretation of the results obtained have been incorporated into this final report following consultation with the sponsor. We are indebted to Nick Jarvis for his valuable contribution.
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EXECUTIVE SUMMARY

The MACRO model is increasingly used to simulate movement of pesticides to surface waters via drainflow and leaching to depth through soils prone to preferential flow. Recent work funded by DEFRA concluded that MACRO is and should continue to be the preferred preferential flow model for regulatory use. However, the predictive use of MACRO is greatly restricted by difficulties in robust parameter selection, particularly as model predictions are significantly affected by changes in many of the problematic parameters. This study aimed to develop guidance on the estimation of those soil hydraulic parameters which describe preferential flow within the MACRO model (version 4.2). The study investigated whether additional field and laboratory measurements could assist in model parameterisation. Work also explored the potential use of inverse modelling techniques to obtain calibrated values for parameters where direct determination did not prove possible.

Total porosity and water content at the micropore/macropore boundary (TPORV and XMPOR)
Comparisons were made between modelling based on standard laboratory determinations and a novel method based on analysis of field moisture contents. It was found that the use of values derived from field data may better represent field conditions.

Tortuosity of the macropore domain (ZN)
This is a very sensitive parameter in determining the relative influence of preferential flow on pesticide transport. Laboratory work with intact soil cores was undertaken to try to measure representative values. However, it was concluded that the direct measurement of the macropore tortuosity term in MACRO is not practicable and that ZN is probably best considered a parameter that has to be systematically calibrated.

Hydraulic conductivity at the micropore/macropore boundary (KSM)
There are existing field protocols for the measurement of this conductivity value as well as a number of pedotransfer functions. Field measurements were made for soils studied in a previous DEFRA-funded lysimeter experiment. Model runs were compared for various values of KSM. Values selected using expert judgement (original simulation) were always significantly smaller than those derived from field measurements or pedotransfer functions, suggesting that they were not physically realistic. Despite this, simulations of pesticide leaching were very much better when KSM values based on expert judgement were used. Here, direct measurement of the parameter adversely affected the quality of the simulation, suggesting that the parameter could have been compensating for processes of importance not
included in the model. Unsaturated hydraulic conductivity is highly variable both spatially and temporally and it is therefore difficult to assign a single measured KSM value, particularly for long-term simulations.

Given the difficulties in independently measuring key parameters, automatic calibration of MACRO (inverse modelling) was undertaken against volumes of leachate and concentrations of a pesticide from a lysimeter experiment to derive values for KSM, ZN and ASCALE (effective diffusive pathlength in soil). A good match between observed and simulated concentrations of pesticide could be obtained in some circumstances, but the optimised parameter values were often not physically realistic and sharply contrasting sets of parameter values achieved a similar fit to the data. These problems arose because: (i) the dataset used had several limitations; (ii) the MACRO model is highly non-linear and exhibits significant correlation between uncertain parameters; and (iii) advanced techniques in inverse modelling (including the use of alternative packages) were not explored. Automatic calibration is a rapidly developing science, but it is considered that the tools are not yet in place to allow robust derivation of input parameters for MACRO on the basis of inverse modelling in the regulatory framework.

It was concluded that it might not always be possible to improve the fit of MACRO 4.2 simulations to measured data by directly measuring more of the variables or through use of inverse modelling. It may thus be more appropriate to select parameters on the basis of generic guidance. Estimation procedures adopted by Cranfield Centre for EcoChemistry are set out and ranges and appropriate values are proposed for 14 key parameters that are primarily related to the description of preferential flow. This guidance is based on application of the model to a number of UK datasets for pesticide leaching (both within PL0538 and in previous projects).
1. INTRODUCTION

Mathematical modelling at a range of complexities has been given a prominent role in the fate and behaviour section of the registration process by Council Directive 91/414/EEC concerning the placing of plant protection products on the market. There is clear evidence to suggest that preferential flow may be an important process for pesticide transport through a wide range of soils including both clays (Johnson et al., 1994; Brown et al., 1995; Harris et al., 1994) and intermediate soils (Aderhold and Nordmeyer, 1995; Flury et al., 1995; Brown et al., 2000a). Preferential flow may result from the presence of macropores (shrinkage cracks and fissures, soil fauna channels, root holes) in structured soils (Beven and Germann, 1982), but also from profile heterogeneities (e.g. horizon boundaries) or water repellency (Hendrickx et al., 1993) in unstructured sandy soils. Relatively rapid movement of water through only a portion of the bulk soil may significantly increase chemical transport by bypassing the soil matrix and decreasing residence time in the upper soil layers where sorption and degradation are generally most important (Brown et al., 2000a).

There has been a rapid development in the simulation of preferential flow over the last 10 years and there has been some incorporation into the regulatory process, particularly at higher tiers of assessment. Deterministic dual-porosity models are the most highly developed at present. The soil porosity is divided into a slow or immobile flow domain (the matrix) and a region of faster flow (the macropores). Examples include CRACK-NP (Armstrong et al., 1995), MACRO (Jarvis, 1994) and RZWQM (Ahuja et al., 1993). Where water in the matrix is immobile, such models are only applicable to heavy clay soils, but a much broader range of conditions can be simulated by including a mechanistic description of slow flow through this domain. For example, MACRO solves the Richards’ equation and convection-dispersion equation in the micropores. Deterministic dual-porosity models are now widely accepted for modelling water flow and solute transport in heterogeneous soils and MACRO is generally used as the regulatory model of choice for preferential flow in Europe. The assumption of a two-domain pore system is a simplification for most soils, but the models have been considered to strike a balance between ease of use and rigour of approach.

Cranfield Centre for EcoChemistry have recently undertaken a review of four preferential flow models for PSD (Beulke et al., 1998; 1999). The reports conclude that the dual-porosity model MACRO should continue to be the preferred preferential flow model for regulatory use. This is because of the model’s broad applicability, user-friendliness and good documentation and the relatively large number of model applications reported in the
literature. MACRO has been coupled to one of the European scenarios to estimate leaching of pesticides to groundwater for regulatory purposes (FOCUS, 2000). It will also be the model used to simulate drainflow for aligned scenarios related to the surface water environment (Russell, 2000).

The MACRO model can be used to describe water and solute transport in a variety of soil types, but the processes of finger flow and funnel flow in coarse-textured soils cannot be simulated. MACRO has been tested against several field and lysimeter studies with a number of different pesticides including dichlorprop and bentazone in Sweden (Jarvis et al., 1994), dichlorprop, MCPA and 2,4-D in Denmark (Miljøstyrelsen, 1994), simazine, methabenzthiazuron and metamitron in Germany (Jarvis, 1995) and chlorsulfuron in Sweden (Bergström, 1996). These evaluations were based on the calibration of a number of parameters and, under these conditions, the model was generally shown to give a reasonable match to observed behaviour. A broad conclusion is that MACRO, in common with other preferential flow models, requires careful calibration before it can be used with confidence as a management tool (Bergström and Jarvis, 1994).

Despite the widespread interest in using MACRO for regulatory purposes, the model remains difficult to parameterise (e.g. Brown et al., 2000b; Beulke et al., 2001). A brief review of literature sources identifying this issue is provided as Appendix 1. Lack of knowledge, inadequate measurement techniques, approximations, inaccuracies and inherent variability result in uncertainty in the selection of values for a significant number of parameters, in common with other environmental fate models. The evaluation of preferential flow models by Beulke et al. (1999) notes that use of MACRO is greatly restricted by difficulties in robust parameter selection, particularly as the model is most sensitive to changes in many of the problematic parameters. This has subsequently been confirmed by a comprehensive sensitivity analysis for MACRO for DEFRA Project PL0532 (Dubus et al., 2000b). A review of research requirements for the further development of preferential flow models identified the most important area for attention as the development of detailed guidance to modellers on how to select ‘difficult’ parameters, particularly those related to preferential flow (Beulke et al., 1999).

The aim of the present study was to address this research need through the development of guidance on parameter estimation for the pesticide-leaching model MACRO (version 4.2). The objectives were:
1. To provide detailed guidance to modellers on how to select ‘difficult’ parameters for the MACRO model (particularly those relating to preferential flow) from readily available information;

2. To provide outline protocols for additional measurements which could be made on experimental soils to facilitate parameter selection for the MACRO model.

The study focuses on estimation procedures for those soil hydraulic parameters used to describe preferential flow and thus required over and above those for chromatographic leaching models such as PEARL, PELMO and PRZM. However, it should be noted that a comprehensive sensitivity analysis for MACRO 4.1 reported by Dubus et al. (2000b) and Dubus and Brown (2002) demonstrated that in most scenarios, predictions by MACRO for pesticide leaching losses were most influenced by parameters related to pesticide sorption and degradation. Under specific circumstances, pesticide-leaching losses were also largely affected by changes in the hydrological properties of the soils which are considered here.

The description of pesticide sorption and degradation in MACRO is relatively simple in the light of the potential for complex interactions between these processes and mass transfer between the four model compartments (micropores/macropores and solid/liquid phases). For example, sorption equilibrium is assumed to be instantaneous and fixed and degradation is characterised as a single, first-order process. Reports in the literature suggest that these simplifying assumptions are not universally valid (Boesten, 2000) and the descriptions of these processes in MACRO should be critically reviewed in cases where degradation and sorption parameters are dominant in determining leaching.

2. **MODEL OVERVIEW**

MACRO is a physically-based preferential flow model that can be used to describe water and solute transport in a variety of soil types, although the processes of finger flow and funnel flow in coarse-textured soils cannot be simulated. The total soil porosity is divided into two flow domains (macropores and micropores), each characterised by a flow rate and solute concentration (Jarvis, 1994). Soil water flow and solute transport in the micropores is modelled using Richards’ equation and the convection-dispersion equation, respectively, whilst fluxes in the macropores are based on a simpler capacitance-type approach with mass flow. In situations where preferential flow is unlikely to occur, the model reverts to the classical solution of Richards’ equation and the convection-dispersion equation. At the surface boundary, the infiltrating water is partitioned between micropores and macropores.
depending on the infiltration capacity of the micropores and the net rainfall intensity. Exchange between micropores and macropores is calculated according to approximate, physically-based expressions using an effective aggregate half-width. A range of bottom boundary conditions is available to the user. Soil temperatures are calculated from air temperatures using the heat conduction equation.

Crop development is based on a simple model which uses dates for emergence, maximum leaf area and harvest. Root depth and crop height are assumed to increase linearly up to the stage where the crop has a maximum leaf area and are then considered constant until harvest. For perennials, the two variables are assumed constant during the simulation. Root water uptake is calculated as a function of the evaporative demand, soil water content and root distribution. Although water uptake can occur in both regions, the water is preferentially extracted from the macropores.

Pesticide degradation is modelled using first-order kinetics. Degradation half-lives need to be specified for the solid and liquid phase of the macropores and micropores, and may be adjusted for temperature and moisture effects. Sorption is assumed to be at instantaneous equilibrium and to be described by a Freundlich isotherm. The magnitude of sorption is assumed to be similar in both pore domains, but the user must specify the distribution of sorption sites between the two. Time-dependent sorption can only be simulated by changing the sorption characteristics at a number of dates during the simulation. MACRO version 4.2 has been used for the current study.

3. THEORETICAL BACKGROUND

3.1 Saturated conductivity (KSATMIN) and boundary hydraulic conductivity (KSM)

Saturated hydraulic conductivity (KSATMIN) and the hydraulic conductivity at the boundary between macropores and micropores (KSM) influence the movement of water through the macropores together with ZN (see Section 3.2). The relationship between hydraulic conductivity in the macropores and soil water content is defined as (under the assumption that shrinkage is not modelled):

\[ K_{ma} = (KSATMIN - KSM) ZN S_{ma} \]  \[ \text{[1]} \]

with
\[ S_{ma} = \frac{\theta_{ma}}{TPORV - XMPOR} \]  \[2\]

where \( KSATMIN \) and \( KSM \) have dimensions of L/T, \( K_{ma} \) (L/T) is the hydraulic conductivity (or water flux density) in the macropore (a function of the degree of saturation in the macropores), \( XMPOR \) (L^3/L^3) is the volumetric water content at the boundary between the two flow domains (when the micropores are saturated and the macropores are empty), \( TPORV \) is the saturated water content (L^3/L^3) and \( \theta_{ma} \) (L^3/L^3) is the volumetric water content in the macropores. Equation [1] provides a description of the \( K-\theta \) relationship in the macropore region and \( ZN \) defines the shape of the curve.

Water movement in the micropores is described using Richards’ equation. This requires information on the relationship between water content and water tension, and between hydraulic conductivity and water tension. Soil water retention in the micropores is calculated using the Brooks and Corey (1964) equation:

\[ \psi = CTEN S_{mi}^{-1/ZLAMB} \]  \[3\]

where \( ZLAMB \) is the pore size distribution index (-), \( CTEN \) is the boundary soil water tension (L) and \( S_{mi} (-) \) is the effective saturation in the micropores given by:

\[ S_{mi} = \frac{\theta - RESID}{XMPOR - RESID} \]  \[4\]

where \( RESID \) is the residual water content (L^3/L^3). The model by Mualem (1976) is used to describe unsaturated hydraulic conductivity in the micropores:

\[ K_{mi} = KSM S_{mi}^{M+2+2/ZLAMB} \]  \[5\]

where \( M \) is the tortuosity factor in the micropores (-).
3.2 ZN

The parameter ZN (tortuosity/pore size distribution factor of the macropores that accounts for macropore size distribution and continuity) is one of the most complicated parameters in MACRO to estimate. Together with KSATMIN, KSM, and soil macroporosity (TPORV-XMPOR), ZN influences the gravity-driven movement of water in the macropores (Eq. [1]). Examples of K-θ relationships in the macropore region for different values of ZN and boundary conductivity (KSM) are shown in Figure 1. With decreasing ZN, the hydraulic conductivity in the macropores at water contents close to XMPOR increases. With decreasing KSM, the conductivity of the micropore region decreases and macropore flow can be initiated at lower rainfall intensities. The importance of preferential flow is thus greater for small ZN and/or KSM values.

![Figure 1. Relationship between the soil hydraulic conductivity and volumetric water content as influenced by ZN and KSM](image)

Beven and Germann (1981) first suggested Eq. [1]. By assuming that the soil is composed of a network of cylindrical vertical pores and partially saturated cracks, Beven and Germann (1981) developed two equations to describe flow (q) as a function of the water content of the macropores (θma). They then plotted q versus θma and approximated the resulting curves with:

\[ q = b \theta^{a}_{ma} \]  \[6\]

where q = Kma of Eq. [1], b (L/T) is a conductance term, θma (L^3/L^3) is the volumetric water content in the macropores, and a is an exponent. Equation [6] is known as the kinematic-
flow assumption (Germann and DiPietro, 1996) due to its similarity to the kinematic wave theory proposed by Lighthill and Whitham (1955). Equations [1] and [6] are equivalent when

\[ b = \frac{\text{KSATMIN} - \text{KSM}}{(\text{TPORV} - \text{XMPOR})^a} \]  

\[ [6a] \]

### 3.3 AScale

Aggregate half-width (ASCALE) controls the movement of water and solute between the micropore and macropore domains. Water exchange $S_w (1/T)$ is treated as an approximate first-order process, neglecting the influence of gravity (Booltink et al., 1993) and assuming a rectangular-slab geometry for the aggregates (van Genuchten and Dalton, 1986):

\[ S_w = \left( \frac{3D_w \gamma_w}{\text{ASCALE}^2} \right) (\text{XMPOR} - \theta_{mi}) \]  

\[ [7] \]

where ASCALE is an effective ‘diffusion’ pathlength (i.e. half the aggregate width - L), $D_w$ is an effective water diffusivity ($L^2/T$) and $\gamma_w$ is a scaling factor introduced to match the approximate and exact solutions to the diffusion problem (fixed to 0.8).

Equation [7] holds if the micropores are unsaturated. If the micropore domain is saturated, flow in the reverse direction (from micropores to macropores) may be generated. This may occur, for example, if micropore hydraulic conductivity decreases with depth in the soil. In this situation, the excess water instantaneously starts to fill the macropores.

The source/sink term for mass transfer of solute between micropores and macropores $U_e$ is given by the combination of a diffusion component (van Genuchten and Dalton, 1986; Valocchi, 1990) and a mass flow component:

\[ U_e = \left( \frac{3D_e \theta_{mi}}{\text{ASCALE}^2} \right) (c_{ma} - c_{mi}) + S_w c' \]  

\[ [8] \]

where $U_e$ has dimensions of $M/L^3T$, $c_{ma}$ and $c_{mi}$ (M/L^3) are solute concentrations in the liquid phase of the macropores and micropores, respectively, and $\theta_{mi}$ is the water content in the micropores ($L^3/L^3$). The prime notation depends on the direction of water flow $S_w$ (i.e. $c' = c_{ma}$ if water flows from macropores to micropores) and $D_e$ is an effective diffusion coefficient ($L^2/T$).
Mass transfer is inversely proportional to the square of the diffusion distance. Hence, AScale is expected to be a sensitive parameter for macroporous soils.

4. DETAILED INVESTIGATION OF SELECTED PARAMETERS

There are four main strategies to derive model parameters: (i) direct measurement; (ii) estimation by curve-fitting from independent experimental data which are not of the same type as those later predicted by the model (e.g., estimation of Brooks and Corey parameters from the water release curve); (iii) back-calculation of key parameters by calibrating the whole model against data which are of the same type as those later predicted by the model (e.g., calibration of parameters determining preferential flow against data on pesticide concentrations in drainflow); and (iv) expert judgement. This section investigates the possibility to directly measure or estimate parameters from independent experimental information. In Section 5, the MACRO model is calibrated against data on the movement of water and solutes through lysimeters from two soils in order to derive key parameters. Generic estimation procedures adopted by Cranfield Centre for EcoChemistry based on experience in the application of the MACRO model to a number of UK datasets for pesticide leaching are presented in Section 6.

4.1 Total porosity and boundary water content

Total porosity (TPORV) and the water content at the boundary between the micropore and macropore regions (XMPOR) have a strong influence on the simulated movement of water and solutes. It should be noted that TPORV refers to the saturated water content, which can be smaller than the total porosity due to trapped air. Often, TPORV is estimated from water release curves measured in the laboratory (water content at zero suction). XMPOR is set to the measured water contents at boundary tension (CTEN) or interpolated between the two points of the water release curve closest to CTEN.

Water release data derived under laboratory conditions may not be fully representative of the relationship between water content and tension in the field. This can be attributed to hysteresis effects or experimental constraints of using a small isolated soil sample. An alternative is to derive TPORV and XMPOR from water contents measured in the field. This may give a better estimate of TPORV and XMPOR than laboratory water retention data. The feasibility of this method was investigated. Data from a field drainflow study (Brown et al.,
were used for this purpose. Volumes of drainflow and associated concentrations of a pesticide were monitored following spring application of the test compound to a clay soil of the Hanslope series (38% clay).

Measured drainflow from 16 May until 16 June 2000 is shown in Figure 2. Measured water contents were available for 19 May 2000 and 30 May 2000 and for three dates when the drains were not running (Figure 3).

On 30 May, drains had been flowing for several days (Figure 2) which suggests that the profile was saturated. TPORV was thus set to the water content measured on 30 May. It was further assumed that drainflow starts when the water content exceeds the storage capacity of the soil matrix. The water content just before the start of a drainflow event thus corresponds
to XMPOR. Ideally, XMPOR should be set to the water content just before drainflow starts. In the absence of additional measurements, XMPOR was set to water contents on 19 May unless the water content was larger than that on 30 May (see Figure 3). In this case, the minimum of all five measurements was used. TPORV and XMPOR values are compared to those derived from laboratory water release curves in Figure 4. TPORV and XMPOR derived from water contents in the field were smaller than those from laboratory water release curves in the topsoil, but larger in the subsoil.

![Figure 4. TPORV and XMPOR values as derived from field measurements (thin line) and from water release data (bold line)](image)

Simulations were carried out with MACRO 4.2 using the two sets of TPORV and XMPOR values. Results are shown in Figure 5 and 6. Drainflow was over-estimated by the model for both parameter combinations. However, concentrations of the pesticide in drainflow were matched better when TPORV and XMPOR values were derived from field water contents (particularly the rapid decrease in concentrations from peak values).
Figure 5. Measured and simulated (MACRO) volumes of drainflow using two sets of values for TPORV and XMPOR (see Figure 4)
Figure 6. Measured and simulated pesticide concentrations using two sets of values for TPORV and XMPOR (see Figure 4)

It should be noted that only TPORV and XMPOR were modified. All other parameters that are linked to TPORV and XMPOR (KSATMIN, KSM, and degradation rate at reference moisture) remained unchanged. The pore size distribution index ZLAMB was assumed to be identical in the field and the laboratory. The changes in TPORV and XMPOR introduce a shift in the water release curve used by MACRO. Figure 7 shows the water release curve for 0-10 cm and 30-38 cm depth before and after changing the saturated and boundary water content.
There is a considerable difference between the two curves over a large range of tensions. Water contents at tensions drier than CTEN cannot be derived from the field study. The validity of the modified water release curve in this range is thus uncertain. It should be noted that the water content at wilting point (WILT) which is used by MACRO to calculate root water uptake was identical for both simulations. This parameter is not calculated by MACRO from the water release curve as the water content at -1500 kPa because (i) this might be inappropriate for some crop/soil combinations; and (ii) errors in the fitted Brooks and Corey curve can be large at large tensions and this may lead to unrealistic calculations for the water content at wilting point (N. Jarvis, personal communication).

Results described above suggest that it may be advantageous to derive TPORV and XMPOR from measurements of soil water contents in the field for modelling pesticide losses in
drainflow from clay and loam soils. It is, however, not clear whether water release curves can be extrapolated to a wider range of water contents. Comparison of measured volumes of drainflow and associated solute concentrations with those simulated on the basis of field values for TPORV and XMPOR should be made wherever possible. In sandier soils, water contents in the field rarely reach saturation and the estimation of TPORV from field data would be difficult.

It may also be possible to derive hydraulic properties of a soil from field leaching studies. Water contents in the field often remain at a roughly constant level throughout winter. It can be assumed that this moisture content corresponds to field capacity of the soil and gives a good indication of the maximum water content in the soil matrix (i.e. XMPOR). Water contents may increase towards saturation for a short time after large rainfall events. The maximum water content reached can be used as an estimate for TPORV, although this will clearly be an effective rather than absolute value. Again, the validity of these parameters and the resulting water release curves should be tested against measured flow and/or solute data where possible.

4.2 Hydraulic conductivity

DEFRA project PL0510 generated data on leaching of a bromide tracer and pesticides including isoproturon (IPU) through lysimeters from five contrasting soils (Brown et al., 1997, 2000a). The ability of MACRO to simulate movement of water and solutes through the lysimeters was evaluated within PL0510 and PL0516 (Beulke et al., 1998). KSM (mm/h) was calculated following the method proposed by Jarvis et al. (1997) which is based on a theoretical relationship between soil pore size distribution and saturated conductivity:

\[
KSM = C \frac{XMPOR}{CTEN^2} \left( \frac{ZLAMB}{ZLAMB + 2} \right) \times 10
\]  

[9]

where \( C \) is a tortuosity parameter set at 183 L^3/T. Beulke et al. (1998) used expert judgement to determine CTEN and obtained XMPOR and ZLAMB from water release curves. Alternatively, the parameters in Eq.[9] can be derived from pedotransfer functions developed by Mayr and Jarvis (1999).

Experience with the MACRO model and communication with the model developer suggested that Eq.[9] may result in an under-estimation of the boundary hydraulic conductivity (which
would in turn over-estimate the importance of preferential flow). In the present project, two alternative approaches to determine KSM were explored for two of the five soils investigated in PL0510 (Sonning series- sandy loam over gravel; and Ludford series- clay loam):

1. Measurements of hydraulic conductivity at -10 cm were made in the field for the Sonning and Ludford soils using tension infiltrometers;

2. KSM was estimated on the basis of pedotransfer functions developed by Jarvis et al. (2002).

The resulting KSM values were used for modelling water and solute movement through the lysimeters. Simulated patterns of leaching were compared to measured data and to the original simulations.

4.2.1 Materials and methods

4.2.1.1 Tension infiltrometer measurements

To determine the MACRO parameter KSM, field infiltration measurements were carried out on two soil series, Ludford and Sonning (Table 1). The purpose of the experiment was to determine the unsaturated hydraulic conductivity of the soils at different tensions. Tension infiltrometers were used (e.g. White et al., 1992; Coquet et al., 2000) and infiltration measurements were made at tensions of -14, -10 and -5 cm. These tensions were selected because they represented different types of pore flows (Ankeny et al., 1991). At tensions greater (drier) than -10 cm, it is assumed that water is mainly moving in micropores, while at tensions lower (wetter) than -10 cm, most of the water moves in macropores (Wilson et al., 1998; Jarvis et al., 2002). The boundary conductivity between the micropores and macropores (KSM) is thus assumed to be at 10 cm.

<table>
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<th>Unit</th>
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<th>Ludford</th>
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<td></td>
<td>Ap 2BCt1 2BCt2 2Cu</td>
<td>Ap 2Bt 2BCt1 2BCt2</td>
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<td>0-28 28-61 61-85 85-122</td>
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<td>$\rho_b$ g/cm³</td>
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<td>Stones %</td>
<td></td>
<td>15.6 31.4 46.2 53.4</td>
<td>- - - -</td>
</tr>
</tbody>
</table>

Table 1. Selected properties of the Sonning and Ludford soils (Beulke et al., 1998)
Tension infiltrometer measurements were made at the soil surface and in the B horizon (approximately 35 cm below the soil surface) of each soil. For each soil/depth combination, two replicated measurements were carried out. For each tension applied, the experiment was terminated when steady-state infiltration conditions were reached. The infiltration rate $Q$ (L/T) was obtained with:

$$Q = \frac{A_c (d_1 - d_2)}{A_{tp} (t_2 - t_1)}$$  \[10\]

where $d_1$ and $d_2$ (L) are the depth of water in the graduated cylinder of the infiltrometer at the beginning and at the end of the infiltration, respectively, $A_c$ (L$^2$) is the surface area of the graduated cylinder, $A_{tp}$ (L$^2$) is the surface area of the tension plate and $t$ is time (T).

By combining the solution for infiltration from a circular source proposed by Wooding (1968) with the assumption that the hydraulic conductivity as a function of tension $[K(h)]$ has an exponential form (Gardner, 1958), $Q$ can be determined by:

$$\ln(Q_h) = \ln \left[ KSATMIN \left(1 + \frac{4}{\pi r \alpha} \right) \right] + \alpha h$$  \[11\]

where $h$ is the applied tension (L), $r$ is the tension plate radius (L) and $\alpha$ (1/L) is a constant from Gardner’s equation:

$$K(h) = KSATMIN \cdot \exp(\alpha h)$$  \[12\]

A plot of $\ln(Q)$ versus $h$ allows for the determination of both $\alpha$ and KSATMIN. The first parameter, $\alpha$, is the slope of the straight line through two points of the graph. Every pair of points (or $h$) yields a different value of $\alpha$, implying that $\alpha$ varies with $h$.

KSM was estimated at $h_{10}$ (a tension of -10 cm). Since three measurements were available ($h_5, h_{10}$ and $h_{14}$), $\alpha$ was calculated for each pair (i.e. $h_5-h_{10}$ and $h_{10}-h_{14}$). The second parameter KSATMIN was determined by using Equation [11] with $h = 0$ (i.e. the intercept of the line on the y-axis) for each pair of points. Equation [12] was then solved twice (once for each $\alpha$-KSATMIN pair), and the average of the two results was taken to characterise KSM. Finally, KSM for each soil/depth combination was taken as the average of the two replicated measurements, unless stated otherwise.
4.2.1.2 *Estimation of KSM from basic soil data*

Pedotransfer functions proposed by Jarvis *et al.* (2002) were used to estimate KSM from basic soil properties:

\[
\log(\text{KSM}) = 0.9396 - 0.018C - 0.01\text{Si}
\]  

[13]

\[
\text{KSM} = 45d_g
\]  

[14]

where \(C\) is the soil clay content (%), \(Si\) is the silt content (%), \(d_g\) is the geometric mean particle diameter, and \(m_i\) and \(d_i\) are the mass fractions and arithmetic mean diameter of particle class \(i\), respectively. Values for \(d_i\) considered were 0.001, 0.026 and 1.025 mm for the clay, silt and sand fractions, respectively (Jarvis *et al*., 2002). There were two limitations in using Eq.[13-15]. The first was that the textural classification in Eq.[13-15] is based on the USDA system, which is slightly different from the one used in particle size analysis of the Sonning and Ludford soil series. The silt fractions range from 2-50 µm and 2-60 µm for the USDA and UK systems, respectively. This implies that some silt particles in the UK scheme would have fallen into the sand category in the USDA scheme. The difference being small, it is assumed here that resulting KSM values will not be affected greatly. The second limitation is that no account is taken of the gravel/stone fraction in Eq.[13-15]. This is a major concern for the Sonning soil which is very gravelly - ranging from 15.6% in the topsoil to 53.4% in the subsoil (Table 1). However, the gravel fraction was not considered in the original determination of KSM so it will be assumed here that ignoring this fraction will not bias the results when compared with original simulations. There is a clear need for pedotransfer functions that account for all particle fractions as they all influence the hydromechanical properties of soils. In the absence of such information, one option to account for the larger conductivity of soil horizons with large stone contents is to shorten the effective horizon depth. For example, a 20-cm layer with 50% stones could be modelled as a 10-cm layer, thereby decreasing the time required for water to travel through the horizon.

\[d_g = \exp(\sum m_i \ln d_i)\]  

[15]

---

1 The factor used in Eq. [4] has been corrected from 45 to 21.3 by Jarvis and co-authors after the work for this project had been carried out. However, the revised KSM values would still be large relative to those selected by expert judgement and results of the modelling would be broadly similar.
4.2.1.3 MACRO simulations

Several MACRO simulations were carried out for both the Sonning and Ludford soils. The first set of simulations aimed at obtaining improved isoproturon (IPU) breakthrough curves from those obtained in an uncalibrated model run performed by Beulke et al. (1998) with MACRO 4.0. Parameter values from Beulke et al. (1998) were used to parameterise MACRO 4.2. Subsequently, KSM values measured in the field were substituted in the MACRO 4.2 parameter file. It is important to note that only KSM was modified and not other parameters closely related to KSM such as CTEN and XMPOR.

In another simulation, field-measured KSM and the KSATMIN values derived from them were substituted. Two additional simulations were carried out using pedotransfer functions developed by Jarvis et al. (2002) to determine KSM. The original parameter files for the Sonning and Ludford lysimeters were derived for MACRO 4.0. For the purpose of this project, these files were converted to MACRO 4.2. MACRO 4.2 differs from version 4.0 mainly in its description of pesticide sorption and solute dispersion. MACRO 4.2 uses the Freundlich sorption isotherm whereas a linear isotherm was used by MACRO 4.0. Tests revealed that the correction for numerical dispersion up to version 4.1 of MACRO was only fully effective for values of the dispersivity more than half the layer thickness. When dispersivity was set to less than half the layer thickness, the effective dispersivity was equivalent to half the layer thickness. In version 4.2, this limitation in the model has been removed as far as is possible. Therefore, the only major changes were (1) the addition of a Freundlich coefficient which was assigned a value of 1 for both soils and (2) the splitting of the first soil layer into two distinct layers of 2 and 5 cm thickness to reduce the pesticide mixing depth and thus increase pesticide leaching responsiveness.

4.2.2 Results

4.2.2.1 Tension infiltrometer measurements

Measurements were successfully conducted for the topsoil of the Sonning and Ludford soils and for the B horizon of the Ludford soil (Table 2). No flow was observed in the B horizon of the Sonning soil for either replicate. Ankeny et al. (1990) reported that initiation of infiltration from infiltrometers varied from 0 to 5 min for soils with high and low infiltration rates, respectively. In this experiment, no infiltration was observed on the Sonning subsoil after a period of 60 min, which was surprising given the coarse texture of the soil. No logical
explanation as to why that happened can be offered. On the other hand, steady-state infiltration conditions were reached after approximately 30 min in the Ap horizon of both soils, but required approximately 90 min in the B horizon of the Ludford, 60 min of which was time before any flow was generated.

Infiltration proceeded at a relatively slow pace, irrespective of the soil or horizon considered. There were differences between replicated measurements (Table 2), but these were considered acceptable given the large variability generally associated with measurements of hydraulic conductivity in the field (e.g. Logsdon and Jaynes, 1996). For example, steady state infiltration rates at \( h_{10} \) were 0.0622 and 0.0889 mm/min (Sonning Ap), 0.0622 and 0.107 mm/min (Ludford Ap) and 0.0133 and 0.0089 mm/min (Ludford B) for replicates 1 and 2, respectively. This resulted in \( K_{10} \) (KSM) values of 1.01 and 1.91 mm/h (Sonning Ap), 0.59 and 1.63 mm/h (Ludford Ap) and 0.20 and 0.33 mm/h (Ludford B) for replicates 1 and 2, respectively (average of KSM determined from \( h_{10}-h_{14} \) and \( h_{5}-h_{10} \)).

As a consequence of the low steady state infiltration rates measured, final steady-state infiltration values were similar at different tensions, some being identical (Table 2). This posed problems in subsequent analysis since identical steady state flow rates at two tensions do not allow for the calculations of \( \alpha \), KSM and KSATMIN between the two tensions concerned (when \( \alpha = 0 \), \( K(h) = KSATMIN \)). This was observed in replicate 2 of both Ap horizons (Table 2). Some instances where infiltration inversions were observed are reported in the literature (Logsdon, 1993; Logsdon and Jaynes, 1996). An inversion takes place when the steady state infiltration rate is larger at greater tensions (say –15 cm) than at lower tensions (say –5 cm). Physically, it is expected that the lower the tension, the more water infiltrates the soil because more pores conduct water. Complete inversions were not observed here but the fact that identical steady state infiltration rates were observed at two different tensions presents a limitation for the methodology.

The hydraulic properties \( \alpha \), KSM (\( K_{10} \)) and KSATMIN used in subsequent MACRO simulations are presented in Table 3. The KSATMIN values were much smaller than those used in the original MACRO simulations by Beulke et al. (1998), the latter values probably being more realistic given the textures of the soils under study (Table 1). Field and laboratory experiments have demonstrated that the hydraulic conductivity close to saturation can increase exponentially for many soils (e.g. Ankeny et al., 1990; Jarvis and Messing, 1995; Moreno et al., 1999). In the calculations carried out above, \( lnKSATMIN \) (and subsequently KSATMIN) was determined by a simple linear interpolation from the straight
line between \( h_{10} \) and \( h_5 \) projected towards \( h_0 \), which is probably the reason for the small calculated KSATMIN shown in Table 3.

Table 2. Steady state infiltration for a combination of soils, horizons and tensions

<table>
<thead>
<tr>
<th>Repetition</th>
<th>Soil/Horizon</th>
<th>( \theta^a )</th>
<th>Steady state infiltration (mm/min) at tensions of:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>%</td>
<td>-14 cm</td>
</tr>
<tr>
<td>I</td>
<td>Sonning Ap</td>
<td>18.5-20.3</td>
<td>0.0533</td>
</tr>
<tr>
<td></td>
<td>Ludford Ap</td>
<td>22.1-24.8</td>
<td>0.0533</td>
</tr>
<tr>
<td></td>
<td>Ludford B</td>
<td>29.2-29.8</td>
<td>N/A</td>
</tr>
<tr>
<td>II</td>
<td>Sonning Ap</td>
<td>20.4-23.1</td>
<td>0.0889</td>
</tr>
<tr>
<td></td>
<td>Ludford Ap</td>
<td>23.6-25.8</td>
<td>0.107</td>
</tr>
<tr>
<td></td>
<td>Ludford B</td>
<td>27.8-30.2</td>
<td>N/A</td>
</tr>
</tbody>
</table>

*Calculated from gravimetric measurements made with on-site samples taken prior to infiltration and using bulk density information from Table 1. No samples were taken in the B horizon of the Sonning, but that horizon was wetter than its A horizon.

Table 3. Results of calculations of KSATMIN and unsaturated hydraulic conductivities at tensions of -14 (K_{14}), -10 (K_{10}) and -5 cm (K_5)

<table>
<thead>
<tr>
<th>Rep</th>
<th>Soil/Horizon</th>
<th>Tensions</th>
<th>( \alpha )</th>
<th>KSATMIN</th>
<th>( K_{14} )</th>
<th>( K_{10} )</th>
<th>( K_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>cm</td>
<td>1/cm</td>
<td>mm/h</td>
<td>mm/h</td>
<td>mm/h</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>Sonning Ap</td>
<td>-14 &amp; -10</td>
<td>2.75E-3</td>
<td>0.757</td>
<td>0.515</td>
<td>0.575</td>
<td>0.660</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-10 &amp; -5</td>
<td>1.08E-2</td>
<td>4.273</td>
<td>0.942</td>
<td>1.451</td>
<td>2.490</td>
</tr>
<tr>
<td></td>
<td>Ludford Ap</td>
<td>-14 &amp; -10</td>
<td>3.75E-2</td>
<td>0.982</td>
<td>0.581</td>
<td>0.675</td>
<td>0.814</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-10 &amp; -5</td>
<td>2.60E-3</td>
<td>0.643</td>
<td>0.447</td>
<td>0.496</td>
<td>0.564</td>
</tr>
<tr>
<td></td>
<td>Ludford B</td>
<td>-14 &amp; -10</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-10 &amp; -5</td>
<td>5.80E-3</td>
<td>0.364</td>
<td>0.162</td>
<td>0.204</td>
<td>0.272</td>
</tr>
<tr>
<td>II</td>
<td>Sonning Ap</td>
<td>-14 &amp; -10</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-10 &amp; -5</td>
<td>9.40E-3</td>
<td>4.880</td>
<td>1.309</td>
<td>1.906</td>
<td>3.050</td>
</tr>
<tr>
<td></td>
<td>Ludford Ap</td>
<td>-14 &amp; -10</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-10 &amp; -5</td>
<td>5.80E-3</td>
<td>2.913</td>
<td>1.293</td>
<td>1.631</td>
<td>2.179</td>
</tr>
<tr>
<td></td>
<td>Ludford B</td>
<td>-14 &amp; -10</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-10 &amp; -5</td>
<td>2.78E-2</td>
<td>5.314</td>
<td>0.108</td>
<td>0.330</td>
<td>1.324</td>
</tr>
</tbody>
</table>

4.2.2.2 MACRO simulations

Sonning
Table 4 lists the KSM and KSATMIN parameter values used in the MACRO simulations for the Sonning soil. Results of the MACRO runs are presented in Figure 8. It is important to note that the original uncalibrated KSM values (run 1) were consistently lower than those derived from field measurements or from pedotransfer functions.
With the original parameter set (modified for version 4.2), MACRO failed to simulate the first IPU peak and although the magnitude of the second peak was well simulated, its occurrence in time was poorly predicted (Figure 8, run 1). Poorer results were obtained after modifying KSM on its own or together with KSATMIN with almost no IPU leaching predicted (Figure 8). The KSM values derived from field measurements were roughly one order of magnitude larger than the original ones (Table 4). From Eq. [1], it can be seen that the higher the KSM value, the lower the water flux in the macropores will be. MACRO results obtained with runs 2 to 5, where KSM was larger than for run 1, yielded consistent results whereby very little leaching of IPU was simulated.

Table 4. Measured and calculated parameters for five MACRO simulations with the Sonning soil

<table>
<thead>
<tr>
<th>Run #</th>
<th>Comments</th>
<th>Parameter</th>
<th>Sonning layers</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>0-31 cm</td>
</tr>
<tr>
<td>1</td>
<td>Original (Beulke et al., 1998)</td>
<td>KSATMIN</td>
<td>54</td>
</tr>
<tr>
<td></td>
<td></td>
<td>KSM</td>
<td>0.309</td>
</tr>
<tr>
<td>2</td>
<td>Field-measured KSM</td>
<td>KSM</td>
<td>1.46</td>
</tr>
<tr>
<td>3</td>
<td>#2 with calculated KSATMIN</td>
<td>KSATMIN</td>
<td>4.27</td>
</tr>
<tr>
<td></td>
<td></td>
<td>KSM</td>
<td>1.46</td>
</tr>
<tr>
<td>4</td>
<td>KSM calculated with Eq.[13]</td>
<td>KSM</td>
<td>3.3</td>
</tr>
<tr>
<td>5</td>
<td>KSM calculated with Eq.[14]</td>
<td>KSM</td>
<td>9.54</td>
</tr>
</tbody>
</table>

Table 5. Measured and calculated parameters for 7 MACRO simulations with the Ludford soil

<table>
<thead>
<tr>
<th>Run #</th>
<th>Comments</th>
<th>Parameter</th>
<th>Ludford layers</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>0-28 cm</td>
</tr>
<tr>
<td>1</td>
<td>Original (Beulke et al., 1998)</td>
<td>KSATMIN</td>
<td>10.34</td>
</tr>
<tr>
<td></td>
<td></td>
<td>KSM</td>
<td>0.14</td>
</tr>
<tr>
<td>2</td>
<td>Field-measured KSM: Rep 1 for surface, average of</td>
<td>KSM</td>
<td>0.508</td>
</tr>
<tr>
<td></td>
<td>reps 1&amp;2 below 28 cm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Field-measured KSM: Rep 2 for surface, average of</td>
<td>KSM</td>
<td>1.6308</td>
</tr>
<tr>
<td></td>
<td>reps 1&amp;2 below 28 cm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Field-measured KSM: Average of both reps at both</td>
<td>KSM</td>
<td>1.0694</td>
</tr>
<tr>
<td></td>
<td>depths</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>#2 with calculated KSATMIN</td>
<td>KSATMIN</td>
<td>0.6428</td>
</tr>
<tr>
<td></td>
<td></td>
<td>KSM</td>
<td>0.508</td>
</tr>
<tr>
<td>6</td>
<td>KSM calculated with Eq.[13]</td>
<td>KSM</td>
<td>2.38</td>
</tr>
<tr>
<td>7</td>
<td>KSM calculated with Eq.[14]</td>
<td>KSM</td>
<td>5.49</td>
</tr>
</tbody>
</table>
Ludford

Table 5 lists the KSM and KSATMIN parameter values used in the MACRO simulations for the Ludford lysimeter. Results of the MACRO runs are presented in Figure 9. Again, the original KSM values were smaller than the measured or estimated ones, but the difference was smaller than for the Sonning soil (Table 5). The use of the original parameters by Beulke et al. (1998) in MACRO 4.2 failed to simulate the first measured IPU peak but matched the second peak fairly well, albeit with a small lag between measured and simulated peaks (Figure 9). With increasing values of KSM (all other runs), MACRO outputs were poorer than with the original run for reasons noted in the previous section. As for the Sonning soil, the smaller, uncalibrated KSM values gave the best match to measured IPU concentrations.
From all the simulations carried out above it can be concluded that the best results were obtained with KSM estimated by the method of Jarvis et al. (1997). The KSM values thus obtained were different from those either measured in the field or calculated using two alternative pedotransfer functions. IPU concentrations predicted by MACRO were highly sensitive to KSM and it is therefore imperative that an appropriate value is specified. It is difficult to reach a conclusion as to which KSM value to use. In this particular example, a reasonable match is obtained between measured and estimated IPU concentrations if the original method is chosen. If field-measured KSM values are used however, poor results are obtained. In this instance, the KSM parameter may have been compensating for processes of importance which are not included in the model. Preferential flow was demonstrated in both soils using dye tracing. In the Sonning soil, this occurred through root channels and around numerous stones present throughout the profile, whereas preferential flow in the Ludford lysimeters was enhanced by a damaged, compacted topsoil. Neither phenomenon is readily simulated by MACRO and this may explain the requirement for an unrealistic value for KSM to best fit the experimental data.

**Results thus imply that providing more accurate parameters through direct measurement will not necessarily improve the quality of the simulation (indeed it may be adversely affected as here).** The problem is compounded by the fact that unsaturated hydraulic conductivity is highly variable both spatially and temporally (e.g. Logsdon, 1993; Logsdon and Jaynes, 1996; Jarvis et al., 1999). It is therefore difficult to assign a single KSM value to a soil series or lysimeter, particularly for long-term simulations. Jarvis et al. (1999) noted that future research should focus on investigating time-varying near-saturated hydraulic conductivity of the soil surface.

All the KSM estimations and calculations derived above were based on the assumption that the boundary tension (CTEN) was −10 cm (or \( h_{10} \)). This cut-off value (determined by expert judgement) may prove inappropriate and may have led to an underestimation of KSM. For example, for a range of soils with textures varying from sandy loam to silty clay, Jarvis and Messing (1995) showed that hydraulic conductivity increased very rapidly between tensions of −5 cm and saturation. For a loamy sand soil, they report CTEN in the vicinity of −6 cm with a corresponding KSM of 1.8 mm/h, while for a sandy loam soil CTEN was −5 cm and KSM was 3.5 mm/h. By changing CTEN from -10 to -5 cm the method of Jarvis et al. (1997) yields KSM values of 1.515, 0.994, 1.237 and 1.016 mm/h for the Ap, 2BC’t1, 2BC’t2 and 2Cu Sonning horizons, respectively. These values are closer to those presented by Jarvis and Messing (1995) for soils with similar textures. It is also apparent from the data presented by Jarvis and Messing (1995) that for the coarser textured soils, changes in \( K \)
between -15 and -5 cm were relatively small. Similar results were reported by Mohanty (1999) for a silty clay loam soil. It is recommended to obtain detailed water retention curves to support the estimation of CTEN.

Figure 9. Observed IPU concentrations as a function of time for the Ludford soil series (filled symbols) and MACRO predictions (open symbol) for runs 1 to 7.
4.3 Estimation of ZN

4.3.1 Experimental measurement

A general method was developed and used by Germann (1985) for the estimation of the parameter \( a \). DiPietro and Lafolie (1991) and Mdaghi-Alaoui and Germann (1998) subsequently used this method. Briefly, the approach consists of applying a pulse of water at the surface of a soil column and monitoring breakthrough of water \( (q) \) at its base. A set of equations that include parameters such as water input, breakthrough of water at the base of the column and time is used to characterise the parameters \( a \) and \( b \) of Eq.[6]. Non-linear regression analysis is then carried out on the falling limb of the drainage hydrograph (graph of \( q \) versus \( t \)) to obtain an estimation of \( a \) (see Germann and DiPietro, 1996 for a more comprehensive description of the method).

As the method described above is cumbersome and not practical as a routine measurement, an alternative approach was used in an attempt to directly measure ZN. An undisturbed soil column (diameter = 20 cm, length = 30 cm, Faulkbourne soil series) was saturated with rainwater, allowed to drain freely, and the amount of water percolating at its base was measured at regular time intervals. The assumption was that over a short time period, the draining water originates from macropores. Using breakthrough information together with KSM and KSATMIN measurements on the column itself, Eq.[1] could be solved for ZN. Unfortunately the swelling potential of the soil upon wetting caused several problems: (i) complete saturation was not reached, (ii) KSATMIN decreased with time due to closure of some pores, and (iii) after long periods with high water contents, the drainage flux was more or less constant with time, indicating that the small amounts of water that were being collected originated from the soil matrix. In response to difficulties encountered in measuring ZN directly, an analysis of previously published data for the parameter was carried out.

4.3.2 Previously published data

Germann and DiPietro (1996) postulated that \( a \) (Eq.[6]) would increase with increasing tortuosity and with increasing dispersive flows. They suggested that if \( 2 < a < 3 \), preferential flow dominated and Eq. [6] could be applied, but if \( a > 10 \) then dispersive flow dominated and the classical theory alone (i.e. Richard’s equation) should be used to model water
movement. There is therefore a ‘grey area’ for $3 < a < 10$ where both preferential and dispersive flows occur.

Several studies have determined the value of $a$ for a variety of natural and artificial soils (Table 6). With the exception of the data of DiPietro and Lafolie (1991), $a$ was higher at low irrigation intensities ($I < 15 \text{ mm/h}$) than at intermediate rates ($15 < I < 100 \text{ mm/h}$). At the higher intensities ($I > 100 \text{ mm/h}$), values of $a$ typically increased. DiPietro and Lafolie (1991) observed that at the lower intensities, the kinematic-wave model failed to reproduce observed breakthrough values adequately for their artificial soil, inducing relatively high values of $a$ at intensities of 33 and 55.6 mm/h. This model failure was shown to be due to dispersion of the macropore wetting front at the lower intensities, a physical phenomenon not accounted for in the kinematic-wave theory. Germann and DiPietro (1999) also provide values of $a$ from a repacked lysimeter experiment. The advantage of this experiment is that the lysimeter was exposed to actual rainfall over a long time period, but the disadvantage is that it was repacked thus destroying any natural structural porosity. The value of $a$ in this experiment ranged from 2 to 2.3 for intensities ranging from 0.36 to 3.6 mm/h, the latter being more realistic than those reported in Table 6.

<table>
<thead>
<tr>
<th>Soil description</th>
<th>$I$</th>
<th>$a$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polyester resin consolidated sand</td>
<td>14.1</td>
<td>3.23</td>
<td>Germann (1985)</td>
</tr>
<tr>
<td></td>
<td>58.3</td>
<td>2.85</td>
<td></td>
</tr>
<tr>
<td></td>
<td>70.6</td>
<td>3.02</td>
<td></td>
</tr>
<tr>
<td></td>
<td>191.5</td>
<td>3.76</td>
<td></td>
</tr>
<tr>
<td>Reconstituted loamy soil</td>
<td>64.8</td>
<td>3.04</td>
<td>Ohashi (1988)$^a$</td>
</tr>
<tr>
<td></td>
<td>56.0</td>
<td>7.28</td>
<td></td>
</tr>
<tr>
<td></td>
<td>126.0</td>
<td>4.41</td>
<td></td>
</tr>
<tr>
<td></td>
<td>770.0</td>
<td>4.36</td>
<td></td>
</tr>
<tr>
<td>Sandy loam surface, sand subsurface</td>
<td>14.8</td>
<td>5.42</td>
<td>Mdaghri-Alaoui and Germann (1998)</td>
</tr>
<tr>
<td></td>
<td>38.2</td>
<td>4.06</td>
<td></td>
</tr>
<tr>
<td></td>
<td>79.2</td>
<td>4.77</td>
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<tr>
<td></td>
<td>82.2</td>
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<td>94.3</td>
<td>4.38</td>
<td></td>
</tr>
<tr>
<td></td>
<td>100.8</td>
<td>5.60</td>
<td></td>
</tr>
</tbody>
</table>


The parameter ZN has been shown to affect solute-leaching predictions with MACRO (Dubus et al., 2000b). Even if ZN could be estimated following the procedure of Germann (1985), it would be likely that a direct comparison between ZN and $a$ is not possible. For
example, Mdaghri-Alaoui and Germann (1998) estimated the parameter $a$ from Eq.[6] and found values ranging from 4 to 6 (Table 6). Mdaghri-Alaoui (personal communication, February 2001) also fitted ZN in MACRO and found a value of 2 for the same soil column. Although the description of soil hydrology in MACRO is more complex and uses more parameters than Eq.[6] to predict flow for the above mentioned experiments, there is a clear discrepancy between the two parameter values. In the first case (using Eq.[6] alone), the value of $a$ would suggest a mixture of preferential flow and dispersive flow, but in the second case (MACRO simulation), the value of ZN would indicate pure preferential flow if the classification of Germann and DiPietro (1996) is used.

The reasons for the observed differences can be explained as follows. Conceptually, Eq. [1] and [6] are equivalent even though they were originally developed from different angles. Equation [1] however explicitly defines the conductance term ($b$) as being the saturated hydraulic conductivity of the macropores while in Eq. [6] the parameter $b$ is a lumped conductivity parameter except for low values of ZN where it is better defined (Germann and DiPietro, 1996). Because of this difference in definition, one could expect differences between ZN and $a$. In addition, with experimental procedures such as that of Germann (1985), outflow from the entire soil column is considered (i.e. both macropore and micropore flow) and this would be reflected in higher values of ZN as some dispersion of the water front takes place in the micropores. However, if the same outflow data are fitted with MACRO, ZN would be smaller as it only applies to the macropore region.

The dependence of $a$ (using Eq. [6]) on rainfall intensity results because dispersion of the water front is accounted for in the procedure of Germann (1985). Capillarity will indeed play a more important role at lower intensities as only the smaller pores will be involved in conducting water. This will also have an impact on ZN as determined in MACRO as only the smaller macropores will be active. ZN is therefore expected to vary with rainfall intensity regardless of the equation used, something not accounted for in MACRO. However, the effect of rainfall intensity on ZN will be smaller than the effect on $a$, because Eq. [1] is only applied to the macropore region.

It can be concluded that it is difficult to derive ZN from independent experimental information. This parameter will remain difficult to parameterise and it is suggested that it be either determined on the basis of expert judgement (see Section 6) or that it be systematically calibrated.
4.4 Dispersivity

During work to produce the FOCUS version of MACRO, it became apparent that the correction for numerical dispersion in MACRO 4.1 was only fully effective for values of the dispersivity more than half the layer thickness. When the dispersivity was set to less than half the layer thickness, the effective dispersivity was equivalent to half the layer thickness. In version 4.2, this limitation in the model has been removed as far as is possible given the numerical solution adopted. The correction for numerical dispersion is now much improved. The effect of dispersivity on model output from version 4.2 was evaluated in a limited sensitivity analysis.

The influence of changes in a large number of model parameters on the leaching of two hypothetical pesticides (Pesticide L, Koc 20 ml/g, DT50 20 days; Pesticide T Koc 100 ml/g, DT50 100 days) through a sandy loam (Wick series) and a clay loam (Hodnet series) was investigated by Dubus et al. (2000b) for MACRO 4.1. The scenarios were modified for use in version 4.2. Dispersivity was initially set to 1 cm. This was then modified to 0.1, 0.5, 2, 5 and 10 times the initial value and simulated pesticide losses four years after a single application were recorded for each of the four scenarios. The results are shown in Figure 10.

Dispersivity influenced the modelling results for Pesticide T in the two soils in opposite directions. In the Hodnet clay loam, a 10-fold increase in dispersivity resulted in a decrease in losses of pesticide T by a factor of 1.5. Preferential flow through macropores is important in this structured soil. At greater dispersivity, the leaching front in the soil matrix is more
diffuse which effectively results in a dilution of concentrations in the upper layer. This decreases the availability of the pesticide for preferential flow and hence total pesticide losses. An increase in losses of pesticide T with increasing dispersivity (factor 1.8) was found in the sandy loam Wick series. Matrix flow is the dominant pathway of flow in the sandy loam soil. Under these conditions, solute breakthrough curves are wider for larger dispersivity and total losses of degrading compounds are generally increased.

There was virtually no effect of dispersivity on losses of pesticide L in the structured Hodnet soil. In contrast, total losses from the Wick soil increased by a factor of 4 when dispersivity increased from 1 to 10 cm. The weaker effect of dispersivity on Pesticide T than on Pesticide L can be attributed to its stronger sorption.

The FOCUS groundwater scenarios workgroup agreed to use a dispersivity of 5 cm for all four models including MACRO. This value seems rather large for simulating soils where preferential flow is an important flow mechanism. Preferential flow causes heterogeneity in the leaching front and this effect encompasses a large proportion of the overall dispersivity of the soil. A value of 1 cm for dispersivity of the soil matrix is recommended in such situations.

4.5 Conclusions on independent estimation of parameters

Dubus et al. (2000b) demonstrated that MACRO, in common with other pesticide fate models, is sensitive to pesticide-related parameters such as Koc and DT50. Input requirements for MACRO with respect to chemical properties are relatively simple and most (but not all) parameters can be measured in the laboratory and/or estimated from field experiments. For soils prone to preferential flow, MACRO was also shown to be sensitive to soil hydraulic parameters which are often more difficult to measure in the field or the laboratory.

TPORV (volumetric water content at 0 kPa) and XMPOR (volumetric water content at the macropore/micropore boundary – i.e. CTEN) are generally derived from water retention curves. An alternative is presented in this report whereby both TPORV and XMPOR are obtained from field measurements of soil water content and drainage events. The water retention curve obtained in this way differed from that generated in the laboratory. The alternative parameter values subsequently used in MACRO had little effect on predictions of drainflow but did improve simulations of associated pesticide concentrations. It is therefore
suggested that TPORV and XMPOR could be assigned values obtained from field-derived water retention data as an alternative to laboratory-derived data. One drawback of the technique is that water contents below CTEN (soil water tension at the macropore/micropore boundary) cannot be obtained.

**KSM** (hydraulic conductivity when the micropore domain is full and the macropore domain is empty – i.e. at CTEN and XMPOR) was evaluated with three methods: based on Eq.[9], using pedotransfer functions (Eqs.[13-15]), and making field measurements. The first method resulted in smaller values of KSM than the two latter ones with the implication that more preferential flow was simulated. This yielded better predictions of pesticide concentrations in the examples considered. It is thought that Eq.[9] artificially underpredicts KSM thereby compensating for processes of importance in the two soils tested which are not included in the model. Although KSM has a clear physical meaning, it may not always be possible to simulate actual leaching behaviour with realistic values. In addition, it must be noted that unsaturated hydraulic conductivity is difficult to measure and exhibits a large spatial and temporal variability. It is therefore difficult to assign a single KSM value, particularly for long-term simulations.

After considering the theoretical background for the origin of **ZN** (tortuosity/pore size distribution factor for the macropores), it is concluded that this parameter is difficult to derive from independent experimental information. ZN is probably best considered as a parameter that has to be systematically calibrated or derived from generic guidance (see Section 6).

The FOCUS groundwater scenarios group recommended that a **dispersivity** of 5 cm should be used for the non-preferential flow models coupled with the scenario shells. For consistency, 5 cm was also used for MACRO simulations with the Châteaudun scenario. In general, a value of 5 cm for dispersivity is rather large for simulating soils where preferential flow is an important flow mechanism. Preferential flow causes heterogeneity in the leaching front and this effect encompasses a large proportion of the overall dispersivity of the soil. A value of 1 cm for dispersivity of the soil matrix is recommended in these situations.
5. CALIBRATION OF KEY PARAMETERS

It was concluded in Section 4 that parameters such as ZN and KSM as used in MACRO may be difficult to measure or estimate independently. Given these difficulties, attempts were made to optimise these parameters by calibrating the whole MACRO model against appropriate data. Results of limited manual calibrations against data on movement of water and isoproturon through lysimeters (PL0510) are presented by Beulke et al. (1999). In this study, a more systematic approach was adopted and automatic calibration was carried out using the inverse modelling software PEST (Doherty, 2000) to derive values for KSM, ZN and ASCALE.

It should be noted that the datasets used in this inverse modelling exercise have some limitations. Both soils exhibited preferential flow phenomena which are difficult to simulate with MACRO. In addition, there were relatively few measurements available and the degradation and sorption properties of isoproturon were not determined in the field soils. However, comprehensive datasets are rarely available for calibration in the regulatory process and the use of the Sonning and Ludford data was deemed acceptable for the purpose of this study.

5.1 Inverse modelling methods

MACRO 4.2 was used in conjunction with the inverse modelling package PEST to derive simultaneously KSM, ZN and ASCALE that were calibrated against data on water percolation and pesticide concentrations for the Sonning and Ludford lysimeters. The parameter ASCALE (effective diffusive pathlength in soil) was included because it is also considered a difficult parameter to estimate. PEST optimises model input parameters to best match model predictions with observed behaviour. This is achieved by minimising an objective function ($\Phi$), defined in PEST as the sum of squared deviations between model-generated observations and experimental observations (Doherty, 2000). Generally speaking, the smaller the objective function, the better the parameter optimisation. In the present case, ASCALE for the top horizon (ASC1), ASCALE for the rest of the soil profile (ASC2), KSM for the top horizon (KSM1) and for the rest of the soil profile (KSM2), and ZN for the entire profile were calibrated using the inverse process. It is important to note that although KSM, ZN and ASCALE play an important role in describing the hydromechanical properties of the soil, other parameters such as potential evapotranspiration also play a significant role. The impact of these parameters was not investigated here.
First PEST optimised these parameters by comparing MACRO predictions for water percolating at the base of the Ludford and Sonning lysimeters with experimental measurements (Beulke et al., 1998). In a second exercise, these parameters were calibrated against measured pesticide concentrations in leachate from the same lysimeters. The same MACRO parameter files described in Chapter 4 were used.

The quality of the sets of optimised parameters was determined by looking at a variety of information generated by PEST (in addition to Φ). These include (Doherty, 2000):

1. Correlation between observed and simulated outputs. The higher the correlation the better the optimisation.

2. Magnitude of the mean value of residuals (MVR = [observed - simulated data]/ number of observations). The optimum value for MVR is 0.

3. Correlation of parameters: if parameters are highly correlated with each other, it may prove difficult to minimise Φ, or many different parameter combinations may yield a similar Φ.

4. Ratio of eigenvalues: if the ratio of the maximum eigenvalue to the minimum eigenvalue is greater than 10^7-10^8 some doubt can be cast as to the appropriateness of the calibrated parameters. Simplifying, an eigenvalue gives information as to the variance in the correlation matrix, the latter consisting of a square matrix representing the correlation between the parameters being optimised in PEST.

Information regarding the PEST/MACRO simulations carried out is presented in Table 7 and in more detail in Appendix 2. The following two subsections provide a general description of the procedures used.
5.1.1 Sonning

For the Sonning lysimeter, a set of PEST optimisations was conducted against measured data on water percolation. A first simulation was conducted with arbitrary but realistic initial values for the parameters to be optimised (Sim 1). A good fit was obtained between measured and simulated percolation. However, Doherty (2000) and Dubus et al. (2000a) warned that for very non-linear formulations such as those found in MACRO, optimisation of parameters can be significantly influenced by starting values supplied at the beginning of the simulation.

A second optimisation (Sim 2) was thus conducted with the original parameter values used in Sim 1 being either halved or doubled. Some of the optimised parameters were different from those obtained with Sim 1. Most criteria chosen to determine the quality of the optimisation indicated that both optimisations were acceptable (Table 7, Appendix 2). The two valid sets of parameters could be deemed acceptable and therefore, five additional PEST simulations were carried out with randomly selected parameter values to investigate the effect of different starting values on parameter estimation. The initial values were generated by the Crystal Ball 2000 software (Decisioneering, 2000) using a Latin Hypercube sampling procedure into a uniform distribution.

Finally, four PEST calibrations were carried out against pesticide concentrations (Sim 8-11). Simulation 8 was with initial parameters of Sim 1 multiplied by two; Sim 9 was with the same initial values as for Sim 2, and Sim 10 was with the same initial parameter values as Sim 3, allowing in both cases a direct comparison between optimisation with water percolation and with pesticide concentration. Sim 11 started with the original parameter values used by Beulke et al. (1998), slightly modified in the subsoil to obtain one average value each of ASC2 and KSM2.
Table 7. Initial and optimised values of parameters used in the inverse modelling procedure and resulting PEST-generated objective function.

<table>
<thead>
<tr>
<th>Identifier</th>
<th>Soil</th>
<th>Criteria</th>
<th>Initial parameters / optimised parameters</th>
<th>Objective funct. ((\Phi))^a</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>ASC1</td>
<td>ASC2</td>
</tr>
<tr>
<td>Sim 1</td>
<td>Sonning Water</td>
<td>10.00</td>
<td>17.63</td>
<td>17.39</td>
</tr>
<tr>
<td>Sim 2</td>
<td>&quot;</td>
<td></td>
<td>5.0</td>
<td>2.5</td>
</tr>
<tr>
<td>Sim 3</td>
<td>&quot;</td>
<td></td>
<td>25.82</td>
<td>15.52</td>
</tr>
<tr>
<td>Sim 4</td>
<td>&quot;</td>
<td></td>
<td>5.472</td>
<td>4.03</td>
</tr>
<tr>
<td>Sim 5</td>
<td>&quot;</td>
<td></td>
<td>1.25</td>
<td>2.77</td>
</tr>
<tr>
<td>Sim 6</td>
<td>&quot;</td>
<td></td>
<td>4.28</td>
<td>11.02</td>
</tr>
<tr>
<td>Sim 7</td>
<td>&quot;</td>
<td></td>
<td>9.52</td>
<td>9.05</td>
</tr>
<tr>
<td>Sim 8</td>
<td>&quot;</td>
<td>IPU conc.</td>
<td>10</td>
<td>5</td>
</tr>
<tr>
<td>Sim 9</td>
<td>&quot;</td>
<td></td>
<td>5</td>
<td>2.5</td>
</tr>
<tr>
<td>Sim 10</td>
<td>&quot;</td>
<td></td>
<td>25.82</td>
<td>15.52</td>
</tr>
<tr>
<td>Sim 11</td>
<td>&quot;</td>
<td></td>
<td>20</td>
<td>5</td>
</tr>
<tr>
<td>Sim 12</td>
<td>Ludford Water</td>
<td>10</td>
<td>6.57</td>
<td>6.48</td>
</tr>
<tr>
<td>Sim 13</td>
<td>&quot;</td>
<td>IPU conc.</td>
<td>10</td>
<td>5</td>
</tr>
<tr>
<td>Sim 14</td>
<td>&quot;</td>
<td></td>
<td>25</td>
<td>60</td>
</tr>
</tbody>
</table>

^aPEST-generated \(\Phi\) can only be compared for identical groups of simulations such as Sonning lysimeter against water percolation.

5.1.2 Ludford

After analysing the results of the PEST optimisations with the Sonning lysimeter, it was decided to carry out only three calibrations with the Ludford soil. One calibration (Sim 12) was against percolation data with parameter values as per Sim 8. The two other optimisations were against pesticide concentrations with (i) the same initial values as Sim 12 (for Sim 13) and (ii) with initial parameter values taken from Beulke et al. (1998) (for Sim 14).
5.2 Inverse modelling results

5.2.1 Sonning

The objective function $\Phi$ will be labelled $\Phi_{\text{wat}}$ when it is calculated for water percolation and $\Phi_{\text{conc}}$ for pesticide concentration. Although PEST generates outputs indicative of the quality of the match obtained against the specific criteria used (water percolation or IPU concentration), information on both criteria can be extracted after each simulation.

All calibrations carried out against percolation data (Sim 1-7) yielded different sets of optimised parameters (Table 7). ASC1 ranged from 4.44 to 670 mm, ASC2 from 1.86 to 232 mm, KSM1 from 0.096 to 0.274 mm/h, KSM2 from 0.0035 to 5.71 mm/h and ZN from 0.92 to 2.46. The variation for ASC1 and ASC2 was much smaller if results from Sim 3 were discounted (i.e. 4.44-17.63 and 1.86-17.39, respectively). In several cases, ZN was less than 2, the theoretical threshold for that parameter Germann and DiPietro (1996).

$\Phi_{\text{wat}}$ was within the range 300-400 for Sim 1 to Sim 3 and 500-700 for Sim 4 to Sim 7, with the best overall $\Phi_{\text{wat}}$ for Sim 3. Unfortunately, Sim 3 which had the lowest objective function also proved to have an unrealistic set of optimised parameters, particularly ASC1 and ASC2. Other information from PEST outputs for the Sonning lysimeter (optimisation against water percolation) were: (i) the eigenvalue ratios were $< 10^7$ in all simulations; (ii) good correlations ($r > 0.85$) were obtained between observed and estimated water percolation; and (iii) the absolute value of mean value of residuals varied from a minimum of 0.39 in Sim 4 to a maximum of 1.63 in Sim 2 (Appendix 2). This information implies that all sets of optimised parameters were deemed adequate. Clearly, although the optimisation was acceptable, the solution was not unique since several sets of parameter values gave similar predictions. Figure 11 shows the best and worst matches obtained for percolation (the selection criterion used was the value of the objective function).
Figure 11. Observed versus measured percolation from the Sonning soil lysimeter after optimisation of ASC1, ASC2, KSM1, KSM2 and ZN with PEST. Sim 3 gave the smallest objective function value and Sim 7 the largest.

Figure 12 shows the corresponding IPU concentrations as predicted by MACRO with the optimised parameters of Sim 3 and Sim 7. For each simulation $\Phi_{\text{conc}}$ was calculated separately (i.e. was not generated by PEST) and resulted in a value of 1582 for Sim 3 and 53300 for Sim 7. IPU concentrations in both simulations were much larger than those generated in Sim 8 to 11 where optimisation was directly against IPU concentrations. Even though, a better match to IPU concentration was obtained with optimised parameters from Sim 3 (with the very large and unlikely values of ASCALE), but in both cases, IPU peaks were vastly over-predicted by MACRO (Figure 12). The large IPU concentrations observed with optimised parameters from Sim 3 and 7 can be explained as follows:

- Sim 3: the large ASC values reduce water movement from macropores to micropores (see Eq. [7]) so more water and pesticide moved in the macropores. This is partly compensated by the relatively large KSM2 (Table 7).
- Sim 7: the value of KSM2 is relatively small thus generating a large amount of macropore flow in the subsoil (Table 7).
Given the above, it is not recommended to optimise parameters against water percolation data alone as $\Phi_{\text{conc}}$ obtained with the original parameter values of Beulke et al. (1998) was much smaller with a value of 141 (before ‘optimisation’), even though simulation results were poor (Figure 8).

In an attempt to further improve parameter optimisation, KSM, ZN and ASCALE were optimised directly against IPU concentrations. These are mainly hydromechanical parameters and it has been demonstrated by Dubus et al. (2000b) that pesticide-related parameters (e.g. Koc and DT50) play a major role in the prediction of solute leaching with MACRO. In the present study, we wanted to test if model predictions could be improved when only a few problematic parameters were optimised against pesticide concentration data.

![Figure 12. Observed versus measured IPU concentrations (Sonning lysimeter) with parameter values for ASC1, ASC2, KSM1, KSM2 and ZN obtained from Sim 3 and 7](image)

Again, different starting values gave different sets of optimised parameters (Table 7). ASC1 ranged from 4.8 to 47.5 mm, ASC2 from 0.32 to 15.5 mm, KSM1 from 0.0042 to 1.6 mm/h, KSM2 from 0.995 to 3.068 mm/h and ZN from 0.67 to 2.92. ZN was less than 2 for three of the four simulations. The quality of the optimised parameters was relatively poor for all simulations with low and/or negative correlation between measured and simulated concentrations and relatively high MVR (particularly for Sim 8 and 9). The smallest overall
Φ_{conc} for the Sonning soil was generated when original values from Beulke et al. (1998) were used as starting values in the optimisation process (Sim 11 in Table 7, Figure 13). This demonstrates the importance of using the best possible estimates of initial parameter values (Doherty, 2000). When the hydrological output was examined, the parameters of Sim 11 gave a relatively poor prediction of percolation with a calculated Φ_{wat} of 881 even though visual observation of Figure 14 shows that the match between measured and estimated water percolation is satisfactory.

Original parameter values in Sim 9 remained unchanged after the PEST optimisation and those of Sim 8 were only slightly changed. This implies that PEST could not find a better set of parameters that would have yielded a lower Φ_{conc}. The selected starting values for these simulations were therefore not adequate for optimisation purposes as Φ_{conc} could be reduced as demonstrated by the results of Sim 11. This is a clear example of the danger of using inverse modelling of very non-linear models, i.e. the outcome is very much dependent on the starting values used. Another issue is that the magnitude of the difference between two Φ_{conc} alone is not sufficient to determine which optimisation is best. Figure 13 shows that almost no IPU leaching was predicted by MACRO in Sim 8, but leaching was predicted in Sim 11. The difference between the two Φ_{conc} is only 27. Care should be taken when analysing such results as Φ_{conc} for Sim 8 was 135 which is the value that is expected if no pesticide concentrations is predicted (i.e. sum of observed concentrations squared). Therefore, although the difference was small, there is no doubt that Sim 11 was somewhat successful which was not the case for Sim 8.

Simulations 9 and 10 (optimisation against IPU concentrations) had identical starting values to Sim 2 and 3 (optimisation against percolation), respectively. Parameters optimised against IPU concentrations were different from those optimised against water percolation, which was expected. The PEST-generated Φ_{conc} was 135 for Sim 9 and the calculated Φ_{conc} was 121 for Sim 2. These numbers are however meaningless since for Sim 9, MACRO predicted almost no IPU leaching throughout the monitored period, while IPU concentrations were actually predicted with Sim 2. For the other set of simulations starting with identical initial parameters, the PEST-generated Φ_{conc} was 114 for Sim 10 and the calculated Φ_{conc} was 1582 for Sim 3.
Calibrations of the MACRO model against data from the Sonning lysimeters sometimes achieved a reasonable match between observed and simulated IPU concentrations (e.g. Sim 11). However, the optimised parameter values were often not physically realistic and sharply contrasting sets of parameter values achieved a similar fit to the data, particularly with regards to the hydrology. In general, it was difficult to achieve a good match to data on both percolation and pesticide concentration. The lowest $\Phi_{conc}$ was obtained when the initial
parameters had been defined according to expert judgement, confirming the importance of supplying the package with the best possible estimate of initial parameter values.

5.2.2 Ludford

Parameter optimisation with PEST for the Ludford lysimeter was not successful when either percolation or IPU concentrations were used (Table 7, Appendix 2). Correlations between measured and estimated IPU concentrations were always low and/or negative. The first optimisation (Sim 12) was carried out against percolation data (Figure 15). The value of $\Phi_{\text{wat}}$ was 2912 and visual inspection of Figure 15 suggests a reasonable match. Most flow peaks were well simulated in terms of magnitude but often were shifted in time when compared to actual measurements, resulting in the large $\Phi_{\text{wat}}$.

![Figure 15. Observed versus measured water percolation in the Ludford lysimeter after optimisation of ASC1, ASC2, KSM1, KSM2 and ZN with PEST.](image)

Optimisations against IPU concentrations yielded poor results as neither the magnitude nor the timing of peak concentrations was matched (Figure 16). This was largely due to the fact that optimisation was carried out for hydromechanical data and that macropore flow was reduced by high KSM values. Better results could probably have been obtained if parameters such as Koc and DT50 had been included in the optimisation process. A MACRO 4.2 simulation with the original parameters of Beulke et al. (1998) is compared in Figure 16 with that of the best PEST optimisation. Visual inspection of the figure would indicate that the original simulation was much better than that of Sim 13, but $\Phi_{\text{conc}}$ for the former (13316) was larger than for the latter (9449). This highlights another danger of using PEST for parameter optimisation. The software aims at minimising $\Phi$ to identify a ‘best’ set of optimised parameters. Using a straight comparison of data points, parameter combinations matching the magnitude but not the exact timing of peak concentrations may be rejected.
For the limited set of simulations carried out for the Ludford soil, PEST was not able to find an adequate set of optimised parameters to match measured IPU concentrations. It is argued here that the original set of parameters was better than the ‘optimised’ ones because peaks of IPU concentration were much better simulated in the former. We attributed equal weighting to all observed concentrations of IPU, but a better match to peak concentrations could have been obtained by giving these measurement greater weight in the calculation of goodness-of-fit.

5.3 Conclusions on calibration of parameters

In response to the difficulty in directly measuring KSM and ZN, an inverse modelling method was used to obtain values for these parameters as well as for ASCALE. For the Sonning soil, the best parameter optimisation was obtained when original parameters used in the optimisation process had been determined by expert judgement. In all cases, several sets of optimised parameter values were obtained for different sets of initial parameter values used in the inverse modelling process. Some of the parameter values obtained were not physically realistic (including some of those from the best optimisation). This demonstrates
the need to restrict the range in parameter values during setup of the optimisation (N. Jarvis, pers. comm.). Most sets of parameters for the Sonning (water percolation) were deemed valid according to indices generated by the software. The difficulties encountered in these calibrations might be attributed to three factors: (i) the dataset used had several limitations; (ii) the MACRO model is highly non-linear and exhibits significant correlation between uncertain parameters; and (iii) advanced techniques in inverse modelling (including the use of alternative packages) were not explored.

Adequate parameter optimisation was not achieved for the Ludford soil, although only three attempts were made. In this instance, minimisation of the objective function $\Phi$ (i.e. sum of squared residuals) for either flow or pesticide concentrations was a limited means to achieve calibration. Flow and, more especially, IPU concentrations showed transient peaks amongst a large number of smaller values. If MACRO simulated these peaks well in terms of magnitude, but at slightly different times (as in the original simulation), $\Phi$ was much larger than if MACRO had not simulated any significant leaching (Sim 13). Preferential flow is by its nature transient, and this is likely to be a significant issue for many attempts to calibrate the MACRO model. A partial solution may be obtained by weighting peaks in flow or concentration deemed to be of particularly significance. A more rigorous approach would be to include the lag between observed and simulated peaks as a parameter to be optimised (i.e. minimised).

It should be noted that the results presented above are for two datasets which had several limitations. There were relatively few measurements for leachate volume and pesticide concentration and the degradation and sorption properties of isoproturon were not determined in the field soil. This makes the robust calibration of input parameters difficult. Inverse modelling with MACRO was carried out successfully for more comprehensive datasets (N. Jarvis, personal communication; Kätterer et al., 2001). Those studies used the inverse modelling tool SUFI. This tool may be less prone to falling into local minima of the objective function.

Given the issues set out above (particularly the complex and non-linear nature of the MACRO model) it is likely that very sophisticated calibration techniques would be required to obtain robust estimates of soil hydraulic parameters. This might involve including a Bayesian component to weight the solution based on prior information on parameter values (and the confidence/uncertainty surrounding that information). Dubus et al. (2002b) have proposed a technique (lattice modelling) to investigate the nature of the lack-of-fit statistic across a defined parameter space in order to identify global minima and investigate
parameter correlation. Automatic calibration is a rapidly developing science, but it is considered that the tools are not yet in place to allow robust derivation of input parameters for MACRO on a routine basis. The technique could be used to investigate potential solutions to parameter estimation rather than to define absolute values for any particular combination of parameters. Important prerequisites of inverse modelling are the availability of a suitable dataset, prior experience with the model and knowledge of the conditions at hand and the ability of the model to simulate the data. A detailed analysis of the use of inverse modelling with pesticide fate models is provided by Dubus et al. (2000a, 2002a).

6. EXISTING PARAMETER ESTIMATION PROCEDURES

Results from Sections 4 and 5 suggest that it may not be possible to parameterise MACRO more accurately simply by directly measuring more of the variables or by calibration. A number of parameters exhibit a large spatial heterogeneity and measured values are uncertain. In addition, a model is only a simplified representation of reality. As a result, parameter values may not only relate to their physical meaning, but may also incorporate either a number of processes or incomplete scientific understanding. It may thus be more appropriate to select parameters on the basis of generic guidance. The text below lists the soil physical and hydraulic parameters required to undertake MACRO simulations and overviews parameterisation procedures adopted by Cranfield Centre for EcoChemistry. These procedures have been developed iteratively over the last 7-8 years of applying MACRO to pesticide leaching/drainflow experiments carried out on a range of UK soils. In some instances, parameters retain their physical meaning, whilst others are treated as lumped parameters that will account for a range of processes and retain only nominal physical meaning. We have tried to develop a framework to limit the range of parameterisation and reduce subjectivity. However, it should be noted that the framework itself is subjective. The text below represents our opinion and one possible way of estimating the necessary soil hydraulic parameters. It should not be considered as definitive or unique. Cranfield Centre for EcoChemistry accepts no liability whatsoever for any use made of the parameterisation procedures described below.

Parameterisation of MACRO is extremely difficult without a measured water release curve for the experimental soil. It is strongly recommended that the curve be measured as a standard component of any study to which the MACRO model is likely to be applied. The inclusion of additional points on the curve between field capacity and saturation is also recommended as this is the critical part of the curve for setting the boundary between
micropores and macropores. In instances where a measured curve is not available, it is probably appropriate to obtain data for a similar soil (e.g. from a soil survey organisation, research institute or previous experiments in the locality).

**KSATMIN**  
*Saturated hydraulic conductivity for the whole soil (micropores and macropores) [mm/h]*

Saturated hydraulic conductivity can be directly measured using a number of approaches applied either *in situ* or to intact soil cores. Laboratory procedures were summarised by Klute and Dirksen (1986) and include the determination of KSATMIN on (preferably) intact soil cores with the constant head and the falling head methods. The former method is easy to use but is only applicable to soils with relatively large conductivities (i.e. approximately between 0.36 and 360,000 mm/h). In contrast, the falling head method is slightly more complicated to use, but is appropriate for soils with lower conductivities (i.e. approximately 36 to 0.0036 mm/h). The main limitations of the laboratory methods pertain to the size of the sample which is relatively small and may not be representative of the field hydraulic regime. To overcome this problem, KSATMIN needs to be determined on a relatively large amount of samples. An advantage is that KSATMIN can be measured for all depth increments used in the MACRO simulation.

Amoozegar and Warrick (1986) listed a number of field methods to estimate KSATMIN. These include the auger-hole and piezometer methods for shallow water tables; and the double-tube and the shallow well pump-in methods (or alternatively the Guelph Permeameter method) for deep water tables. These methods are more cumbersome to implement than the laboratory methods and have the same problem of representativeness of field conditions. Moreover, it is more difficult or even impossible to determine KSATMIN for different soils layers.

In the absence of measured data, algorithms to estimate saturated hydraulic conductivity have been reported by Hollis and Woods (1989) (Figure 17). A large number of values for KSATMIN and other soil hydraulic properties can be found in international and national databases (e.g. Wösten *et al.*, 1994; Leij *et al.*, 1996). Generic values based on broad soil texture classes have been proposed by Tikta et al. (2000).
Figure 17. Flow chart for the determination of KSATMIN (after Hollis and Woods, 1989). AC is the aeration capacity, and $\theta_{0kPa}$ and $\theta_{5kPa}$ are the soil volumetric water contents at pressures of 0 and 5 kPa, respectively. $\theta_{0kPa}$ can be calculated with $(1-(BD/PD))x100$ where BD and PD are bulk and particle densities, respectively.

KSATMIN = 8.03578 - (6.7707xAC) + (0.833xAC$^2$) if AC < 7.5%

KSATMIN = 5.8521 - (5.4125xAC) + (1.05138xAC$^2$) if AC < 4%

KSATMIN = 0.4535 x AC$^{1.03423}$ if % Cl < 16 and % Si + 2 x % Cl < 31 and AC < 7.5%

KSATMIN = 0.14143 x exp(AC x 0.46944) if % Cl < 16 and % Si + 2 x % Cl < 31 and AC < 4%
FRACMAC  The fraction of total sorption sites in the macropore domain [-]

This parameter cannot be measured, but reasonably robust values may be estimated on the basis of soil type.

Range: 0.01 - 0.04

Suggested values: Sand, sandy loam, loam  0.04
                  Clay loam           0.02
                  Clay              0.01

CTEN  Soil water tension at the boundary between micropore and macropore domains [cm].

As described in Section 4.2, physically this parameter can be expected to take a value of ca. 10 cm in most soils. In simulating a range of predominantly UK soils, we have successfully used the CTEN parameter in combination with the equation to estimate KSM described below as a means to approximate the relative extent of preferential flow. **It should be noted that the suggested values below (and their impact on the estimation of KSM) do not have direct physical meaning.** These two parameters act here as lumped values indicative of the overall likely impact of preferential flow. The clay content of the soil is used as the principal factor determining extent of preferential flow.

Range: 10-50 cm (i.e. -1 to -5 kPa)

Suggested values: Clay content (%)  CTEN (cm)
                  <10            10
                  10-15          12
                  15-20          15
                  20-25          18
                  25-30          25
                  30-35          30
                  35-45          40
                  >45           50
Particle size within the sand fraction is also of importance. A CTEN value of 10 cm is adequate for coarse sands, whereas 20 cm may be a more appropriate setting for medium sands and a value of 30-40 cm should be used for fine sands (N. Jarvis, pers. comm.).

It may be possible to estimate CTEN by analysing the shape of the water release curve. A breakpoint in the water release curve should be visible at CTEN for soils with a distinct bimodal structure. However, the methodology to determine water contents is often not identical over the whole range of tensions. This might introduce an artificial breakpoint in the water release curve.

**KSM**

**Hydraulic conductivity when the micropore domain is full and the macropore domain empty (i.e. at CTEN and XMPOR) [mm/h]**

This parameter can be measured using tension infiltrometry as discussed in Section 4.2.1.1 or estimated using the pedotransfer function of Jarvis *et al.* (2002). In simulations for this and other research projects, we have found that smaller values of KSM than those yielded by either method give better simulations of observed behaviour. The parameter is probably compensating for processes not included in the model. Our solution is to artificially increase CTEN according to soil type (i.e. move further away from saturation) and use the equation proposed by Jarvis *et al.* (1997) to assign KSM (the approach implies that both KSM and CTEN must then be viewed as lumped parameters with only nominal physical meaning):

\[
KSM = 1830 \frac{XMPOR}{CTEN^2} \frac{ZLAMB}{ZLAMB + 2}
\]

**Range:**

0.03 - 2.00

**Suggested topsoil values:**

- Sand: 0.8
- Sandy loam: 0.6
- Loam: 0.3
- Clay loam: 0.15
- Clay: 0.05
ZN  Tortuosity/pore size distribution factor for the macropores [-].

As described in Section 4.3, ZN is difficult to derive from independent information. Although measurements of ZN as a function of soil type and rainfall intensity have been made, these are primarily on artificial soils and are almost certainly beyond the scope of most parameterisation exercises. ZN can effectively be used within MACRO with rather a small range and with actual value determined by anticipated pore geometry.

Range: 2 - 4 (exceptionally values to a maximum of 6)

Suggested values:
- Distinct bimodal pore system (clays, certain coarse sands) 2
- Graded pore distribution (sandy loams, other light loams) 4

Situations between these two extremes would take intermediate values of ZN.

ZLAMB  The pore size distribution in the micropore domain [-].

This parameter is best estimated by fitting the Brooks and Corey equation to the measured water release curve. All points on the curve wetter than CTEN (the boundary between micropores and macropores) should be omitted before fitting. It is important to obtain a good fit to the water contents close to the boundary between the soil matrix and the macropores. Often, the fit can be improved by omitting the water content at wilting point.

Range: 0.1 - 0.4

Suggested topsoil values:
- Sand 0.3
- Sandy loam 0.2
- Loam 0.18
- Clay loam 0.15
- Clay 0.12

GAMMA  Bulk density [g/cm³]

Use measured value for intact soil cores.
TPORV  Volumetric water content of saturated soil (i.e. 0 kPa) [%]

Either take the value from the measured water release curve or derive an effective field value on the basis of monitoring for field moisture contents as described in Section 4.1. Note, this parameter is not the total porosity of the soil. Total porosity is often derived from soil bulk density and the density of major soil constituents. The result can be reduced by 1-2% to account for trapped air at saturation.

XMPOR  Volumetric water content at the boundary between micropore and macropore domains (i.e. CTEN) [%]

Either take the value from the measured water release curve or derive an effective field value on the basis of monitoring for field moisture contents as described in Section 4.1.

WILT  Volumetric soil water content at wilting point [%].

Take value from the measured water release curve at -1500 kPa.

RESID  Residual water content [%]

In theory, this is the water content at which conductivity is considered negligible. It is usually acceptable to set this parameter to zero unless simulating a detailed field experiment.

ZP  Slope of the shrinkage characteristic [-].

This parameter is used to describe shrink-swell of clay-rich soils in response to wetting and drying cycles and will alter the macroporosity with soil moisture status. In general, soils subject to significant shrinkage will be prone to preferential flow even when fully wetted and it is probably acceptable (and certainly more robust) to set this parameter to zero.
ZA Exponent in the hydraulic conductivity - macroporosity relationship [-].

This parameter is not relevant if ZP is zero and can be left at the default of 1.0.

ASCALE The effective diffusive pathlength in the soil [mm]. This value determines the rate of transfer of water and solute between the micropore and macropore domains.

If there is a description of soil structure for the soil, ASCALE may be derived in a consistent manner using the relationships proposed by Jarvis et al. (1997) with the size and shape of aggregates and degree of structural development (FAO, 1990).

<table>
<thead>
<tr>
<th>Size</th>
<th>Shape</th>
<th>Granular</th>
<th>Platy</th>
<th>Blocky</th>
<th>Prismatic</th>
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<td>2</td>
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<td>Very coarse</td>
<td></td>
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</table>

Multiplication factors for degree of structural development:

- Very weakly or weakly developed 1.0
- Moderately developed 2.0
- Strongly or very strongly developed 3.0

Structureless - effective diffusion pathlength = 1 mm (nominal zero)

Often, we will limit the range for ASCALE to 5 - 150 mm. Soil is often described as structureless if it either consists of single grains (e.g. deep subsoil in a sand) or if the structure is massive (e.g. a compacted layer in a clay). For the former, we would set a small value for ASCALE and for the latter a large value (e.g. 100 mm).

In the absence of a description of soil structure, it might be useful to examine values of ASCALE for similar soils in MACRO_DB. The topsoil value is the most important. For a ploughed topsoil, representative values range from 10 to 100 mm although values of 10 mm
(poorly structured soils), 20 mm (moderately structured soils) and 30 mm (strongly structured soils) may form a useful starting point. ASCALE will often tend to remain constant or decrease with depth in sands and light loams. Conversely, ASCALE will often tend to increase with depth in medium loams and clays.

7. CONCLUSIONS

Owing to its broad applicability, user-friendliness, good documentation, and the relatively large number of applications reported in the literature, MACRO remains the preferred dual porosity model for the prediction of water percolation and solute transport in the vadose zone. However, MACRO is relatively difficult to parameterise and simulated outputs are sensitive to several ‘problematic’ parameters. This research project aimed at providing guidance for the determination of these parameters.

- Field methods for determining TPORV and XMPOR were presented and results obtained with these parameter values compared favourably with measured pesticide concentrations. However, this method only provides partial information as to the relationship between soil volumetric water content and water tension and can only be used as a complement to laboratory-derived water retention curves.

- It is concluded that ZN is difficult to measure through independent experimentation. KSM can be measured relatively easily, but resulting values did not improve the accuracy of the simulations considered here. The parameter was probably compensating for processes not included in the model. Difficulties were also encountered in parameterisation using inverse modelling. In these circumstances, selection of values on the basis of general guidance may be the most transparent approach.

- Finally, it is recommended that a value of 1 cm be assigned for dispersivity of the soil matrix for soils with dominant bypass flow.

MACRO remains a model that is difficult to parameterise and use in conjunction with standard scenarios may offer the best potential to investigate the impact of preferential flow on leaching of pesticides. It is likely that values for some parameters must be derived by expert judgment. MACRO should thus be used with great care as a predictive tool as many of the problematic parameters are both greatly uncertain and can significantly influence model outputs.
8. REFERENCES


APPENDIX 1. LITERATURE COMMENTS ON THE PREDICTIVE SIMULATION OF MACROPORE FLOW


[Discussing the decision on whether or not to include a groundwater scenario with macropore flow]:
"The question of macropore flow was discussed at length. The main reason for including it is that macropore flow can be an important process, especially in structured soils. Macropore transport is more affected by site characteristics and less by compound-specific properties than chromatographic flow. Reasons for not considering macropore flow would include:

- although great progress has been made in the past few years, current estimation procedures for crucial macropore flow parameters are not yet sufficiently robust in comparison to chromatographic flow models
- few of the normal regulatory models consider macropore flow, and
- sensitive sites for chromatographic flow are usually not the sites most sensitive to macropore flow (sites most sensitive to macropore flow are often finer-textured soils with drainage systems)."


"Outputs from the macropore flow models MACRO and CRACK-P are sensitive to parameters related to the macropore region (e.g. macropore conductivity, volume, spacing), which are, in turn, difficult to estimate. This may lead to high levels of predictive uncertainty, compared to the use of models in non-structured sandy soils."


"Current models that consider macropore flow require that soil parameters be obtained by calibration. More advances are required before predictions of macropore flow can be made using soil parameters in existing data bases."

"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. 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."


"Nofziger *et al.* stressed that 'Although models exist which incorporate preferential flow, the independent determination of the soil parameters which describe these pore level processes is a major challenge to users of those models.' Such models will certainly need careful calibration for a variety of benchmark soil types and climates before they can be used with confidence as management tools."
## APPENDIX 2. OPTIMISED PARAMETER VALUES OBTAINED WITH PEST

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<th>Criterion</th>
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<th>Final</th>
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<th>Highest $r^a$</th>
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<th>$\lambda$ ratio$^d$</th>
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<td>IPU conc.</td>
<td>ASC1 = 10, ASC2 = 5, KSM 1 = 3.2, KSM 2 = 2, ZN = 2</td>
<td>ASC1 = 10, ASC2 = 10.51, KSM 1 = 1.345, KSM 2 = 3.068, ZN = 0.67</td>
<td>-0.43</td>
<td>1.81</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Sim 9</td>
<td>&quot;</td>
<td>&quot;</td>
<td>ASC1 = 5, ASC2 = 2.5, KSM 1 = 1.6, KSM 2 = 1, ZN = 1</td>
<td>ASC1 = 5, ASC2 = 2.5, KSM 1 = 1.6, KSM 2 = 1, ZN = 1</td>
<td>-0.28</td>
<td>1.81</td>
<td>0.91</td>
<td>ASC1 &amp; ASC 2 &amp; KSM 1 &amp; KSM 2</td>
<td>356</td>
</tr>
<tr>
<td>Sim 10</td>
<td>&quot;</td>
<td>&quot;</td>
<td>ASC1 = 25.82, ASC2 = 15.52, KSM 1 = 0.06, KSM 2 = 0.22, ZN = 0.87</td>
<td>ASC1 = 47.5, ASC2 = 15.46, KSM 1 = 0.23, KSM 2 = 2.22, ZN = 1.43</td>
<td>-0.079</td>
<td>1.02</td>
<td>≥±0.9</td>
<td>KSM 2 &amp; ASC 2 &amp; KSM 2 &amp; ZN &amp; ASC 1 &amp; ASC 1</td>
<td>4,515</td>
</tr>
<tr>
<td>Sim 11</td>
<td>&quot;</td>
<td>&quot;</td>
<td>ASC1 = 20, ASC2 = 5, KSM 1 = 0.309, KSM 2 = 0.22536, ZN = 4.5</td>
<td>ASC1 = 4.8, ASC2 = 0.32, KSM 1 = 0.042, KSM 2 = 0.995, ZN = 2.92</td>
<td>0.022</td>
<td>0.97</td>
<td>&gt;0.93</td>
<td>ASC 2 &amp; ASC 2 &amp; ASC 1 &amp; ZN</td>
<td>3,327</td>
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<td>Identifier</td>
<td>Soil</td>
<td>Criteria&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Initial</td>
<td>Final</td>
<td>r</td>
<td>MVR&lt;sup&gt;β&lt;/sup&gt;</td>
<td>Highest r&lt;sup&gt;2&lt;/sup&gt;</td>
<td>Parameters w/ highest r</td>
<td>λ ratio&lt;sup&gt;δ&lt;/sup&gt;</td>
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<tr>
<td>Sim 12</td>
<td>Ludford</td>
<td>Water</td>
<td>ASC1 = 10</td>
<td>ASC1 = 6.57</td>
<td>0.41</td>
<td>-0.53</td>
<td>0.84</td>
<td>ASC 2 &amp; KSM 1</td>
<td>25.7</td>
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<td>ASC 2 = 5</td>
<td>ASC 2 = 6.48</td>
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<td>KSM 1 = 3.2</td>
<td>KSM 1 = 0.82</td>
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<td>KSM 2 = 6.48</td>
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<td>ZN = 2</td>
<td>ZN = 3.84</td>
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<td>Sim 13</td>
<td>&quot;</td>
<td>IPU Conc.</td>
<td>ASC1 = 10</td>
<td>ASC1 = 4.76</td>
<td>-0.56</td>
<td>9.74</td>
<td>&gt;±0.9</td>
<td>KSM 2 &amp; ZN</td>
<td>115,376</td>
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<td>ASC 2 = 5</td>
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<td>ASC 1 &amp; KSM 1</td>
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<td>KSM 1 = 3.2</td>
<td>KSM 1 = 5.34</td>
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<td>ASC 1 &amp; KSM 2</td>
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<td>KSM 2 = 2</td>
<td>KSM 2 = 4.85</td>
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<td>KSM 1 &amp; KSM 2</td>
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<td></td>
<td>ZN = 2</td>
<td>ZN = 0.4</td>
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<td>Sim 14</td>
<td>&quot;</td>
<td>&quot;</td>
<td>ASC1 = 25</td>
<td>ASC1 = 7.71</td>
<td>-0.43</td>
<td>12.4</td>
<td>&gt;±0.9</td>
<td>ASC 1 &amp; ZN</td>
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<td>ASC 2 = 60</td>
<td>ASC 2 = 19.38</td>
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<td>KSM1 &amp; ZN</td>
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<td>KSM 1 = 0.14</td>
<td>KSM 1 = 1.02</td>
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<td>ASC 1 &amp; KSM 1</td>
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<td>KSM 2 = 0.2325</td>
<td>KSM 2 = 0.066</td>
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<td>ZN = 4.5</td>
<td>ZN = 10.25</td>
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</table>

<sup>a</sup>Criteria used to optimise parameters. There were two possibilities: optimisation against volumes of leachate or pesticide concentrations.

<sup>β</sup>Mean value of residuals. The closer this number is to zero the better.

<sup>2</sup>Highest correlation between optimised parameters. The lower the value the better.

<sup>δ</sup>Ratio of the highest to the lowest eigenvalue. Results deemed acceptable (pending other criteria) if ratio < $10^7$-$10^8$. 