INCORPORATING MACROPORE FLOW INTO FOCUS PEC MODELS

JARVIS N.[1], BOESTEN J.[2], HENDRIKS R.[2], KLEIN M.[3], LARSBO M.[1], ROULIER S.[1], STENEMO F.[1], TIKTAK A.[4]
[1]Department of Soil Sciences, SLU, Box 7014, 750 07 Uppsala, Sweden
E-mail. Nicholas.Jarvis@mv.slu.se
[2]Alterra, Wageningen University & Research Centre, PO Box 47, 6700 AC Wageningen, The Netherlands.
[3]Fraunhofer Institute for Environmental Chemistry & Ecotoxicology, Auf dem Aberg 1, 57392 Schmallenberg, Germany.
[4]RIVM, PostBus 1, 3720 BA, Bilthoven, The Netherlands.

ABSTRACT
Macropore flow can strongly influence leaching of pesticides in the unsaturated zone, but this process has until now played only a limited role in exposure assessments. This paper describes efforts to incorporate descriptions of macropore flow into the exposure assessment models PEARL and PELMO, recommended for use in pesticide registration in the EU. We also outline improvements made to an existing macropore flow model (MACRO), including upgraded numerical routines, new processes (e.g. tillage, kinetic sorption), and an inbuilt inverse modeling capability (SUFI) to help parameterization. Simulations made with the macropore flow version of PELMO and the existing FOCUS version of the model are compared with measurements of pesticide leaching made in two clay soils (Lanna, Andelst). Results show that the functional description of macropore flow included in PELMO appears promising, and should be further tested on additional high quality datasets. Use of SUFI to estimate parameters in MACRO 4.3 and 5.0 for the Lanna dataset, showed that the effects of differences in parameter optimisation methods were overshadowed by differences between models in process descriptions and numerical methods. Despite the comprehensive nature of the dataset, one important parameter regulating the strength of macropore flow could only be identified with a large uncertainty.

KEYWORDS: macropore flow, model, FOCUS, PEARL, MACRO, PELMO

INTRODUCTION

The heterogeneity of undisturbed soils in the field often leads to markedly non-uniform patterns of water flow and agrochemical displacement, invalidating the chromatographic transport theory that underlies most leaching models currently used for pesticide exposure and risk assessment. Preferential flow is the generic term used to describe this irregular wetting. It is an umbrella term, covering several processes with different physical causes, but with the common feature that non-uniform wetting leads to an increase of the effective velocity of the water flow through a small portion of the soil unsaturated zone. Structural macropores represent high-conductivity flow pathways that by-pass the less permeable soil matrix (Beven and Germann, 1982). Preferential flow also occurs in unstructured sandy soils in the form of unstable flow or fingering caused by profile heterogeneities such as horizon interfaces or water repellency (Hendrickx et al., 1993), or simply as heterogeneous flow in soils characterised by mixtures of materials of differing texture and pore size distribution (Roth, 1995). Preferential flow greatly increases the risk of leaching of surface-applied agrochemicals to groundwater and surface waters bodies (Jarvis, 2002), since infiltrating water is channeled through only a small fraction of the total pore space, at rates which are too fast to allow sufficient time for equilibration with slowly moving 'old' water stored in the bulk of the soil matrix. Thus, the sorption and degradation capacity of the topsoil is quickly 'by-passed' and a significant fraction of the pesticide reaches subsoil layers where these attenuation processes are generally less effective. Nevertheless, despite its potential significance, preferential flow models currently only have a limited role in EU exposure assessments for groundwater (FOCUS, 2000), but will play a more prominent role in surface water assessments. This is mainly because macropore flow is considered to be primarily an important process for movement of pesticides to drainage systems in fine-textured soils (FOCUS, 2001). This paper describes new modules for preferential flow that are being incorporated into two models used in EU pesticide regulation (PELMO and PEARL). This paper also briefly presents improvements to the current process descriptions in an existing macropore flow model (MACRO) that is currently used for pesticide regulation in the EU.

MODEL IMPROVEMENTS

In the following sections, each of the FOCUS regulatory models is briefly described, and the methods adopted to include descriptions of macropore flow in the models are presented.

The PEARL model

The PEARL model of pesticide fate and transport is based on the convection-dispersion equation. It requires values of water flow and water content, which must be simulated with a separate water balance model. Currently, the model SWAP (van Dam, 2000), based on Richards equation, is used to supply this 'driving data'. The SWAP model is being modified to account for macropore flow by introducing an adapted version of the FLOCR model (Hendriks et al., 1999). Two types of macropore are included: a permanent static macropore volume independent of the soil moisture status and dynamic shrinkage cracks whose volume depends on the shrinkage characteristic and the current soil moisture content. Furthermore, two classes of macropore are distinguished with respect to pore continuity, one domain continuous throughout the profile, and one domain representing macropores ending at different depths in the profile, resulting in 'internal catchment'. Water enters the macropores at the soil surface either as rain falling directly into the macropores or as 'runoff' if the rainfall rate exceeds the infiltration capacity of the matrix. Water flowing into the macropores accumulates at the bottom, while uptake into the matrix takes place only in the saturated part of the macropore. Pesticide is introduced into the macropores using the mixing cell concept (Jarvis, 1994). It is assumed that the two classes of macropore each have a uniform pesticide concentration (assuming perfect mixing and ignoring adsorption and transformation). Uptake of pesticide from macropores into the matrix is calculated as the product of the water uptake rate and the pesticide concentration in each of the two macropore domains. At the time of writing, the coding of these new routines is not complete, so that it is not yet possible to present comparative simulation results.

The PELMO model

The PELMO model (Klein, 1995) uses a 'tipping bucket' approach to describe water flow, and the convection-dispersion equation for solute transport. In a functional model like PELMO, there is little sense in incorporating a mechanistic description of preferential flow. Therefore, a simple functional approach to bypass flow has been adopted whereby infiltration is partitioned between matrix and macropores using a simple 'two-parameter' linear response model with a threshold :

$$I_{ma} = 0, \quad I_{mi} = R \quad ; \quad R \leq I_c$$
$$I_{ma} = f(R - I_c), \quad I_{mi} = (1 - f)(R - I_c) + I_c \quad ; \quad R > I_c$$

where I_c is the threshold daily rainfall amount which generates infiltration into macropores, and *f* is the fraction of the excess rainfall which is routed into macropores. The concentration of pesticide entering the macropores at the soil surface c_{ma} is calculated using the mixing depth concept, whereby incoming rainfall is assumed to mix perfectly with the resident water in a shallow surface layer of soil (Jarvis, 1994):

$$Q_1\left(\frac{z_d}{\Delta z}\right) = c_{ma}\left(R + z_d\left(\theta_{mi} + \gamma\, k_f\, c_{ma}{}^{n-1}\right)\right)$$

where z_d is the mixing depth, Δz is the thickness of the top numerical layer, Q_l is the amount of pesticide stored in the top numerical layer, R is the rainfall amount, θ_{mi} is the matrix water content, γ is the bulk density and k_f is the Freundlich sorption coefficient. The flux of pesticide into the macropores is given by c_{ma} multiplied by the infiltration rate into macropores I_{ma}, and this amount of pesticide is extracted from the matrix to maintain the mass balance.

As with PEARL, water flow in macropores is not explictly modelled. Water and pesticide moving in macropores are assumed to be taken up into the matrix at a user-defined depth corresponding to the base of the macropores. This functional approach requires four additional parameters compared to the existing version of the model.

In this paper, both the new version of PELMO including preferential flow, and the existing FOCUS version of PELMO are compared to data on pesticide concentrations in drainflow from two structured clay soils, at Andelst, Netherlands (imidacloprid) and at Lanna, Sweden (bentazone). No calibration of the pesticide parameters, or the parameters describing the soil matrix was performed. For the macropore flow version of the model, the mixing depth was set to 5 cm, while the other three parameters (depth of macropores, threshold rainfall, and fraction of excess rainfall entering macropores) were estimated by 'trial and error' calibration.

The MACRO model

MACRO is the most widely-used example of the type of preferential flow and transport model that is usually termed 'dual-permeability'. The soil pore system is divided into two parts, one part with a high flow capacity and low storage capacity (macropores) and the remainder with a low flow capacity and a high storage capacity (micropores). The boundary between the pore regions is defined by a fixed water tension, and corresponding water content and hydraulic conductivity. Classical continuum equations are used to model flow and transport in the micropores (Richards equation and the convection-dispersion equation) while flow in the macropores is calculated using the kinematic wave equation (Germann, 1985), assuming gravity-dominated flow (i.e. neglecting capillarity). Transport in macropores is calculated neglecting dispersion-diffusion, but accounting for adsorption by one parameter that partitions the sorption constant between the two flow regions. The concentration of pesticide entering the macropores at the soil surface is calculated using the mixing depth concept outlined above. Mass exchange between the two pore regions is calculated using approximate first-order equations based on an effective diffusion pathlength, accounting for both convection and diffusion. Internal catchment can be modelled by setting the macroporosity and macropore conductivity to very small values at a given depth in the soil, but this cannot be combined with macropores that are continuous throughout the profile, since only one macropore domain is considered in MACRO.

A new version of MACRO (5.0) has been developed that includes several improvements:

1.) the numerical routines have been upgraded, by converting to implicit solution methods for water and heat flow and solute transport, which in turn allows for a larger number (up to 200) of much thinner layers in the profile.
2.) van Genuchten (1980) hydraulic functions are used instead of Brooks-Corey. This was prompted by the change in numerical methods described above, but it also allows more flexibility in matching measured soil hydraulic properties. However, it requires one additional parameter, since the boundary between macropores and micropores is no longer given automatically by the Brooks-Corey air entry pressure.
3.) the effects of tillage practices, and subsequent soil sealing, on soil structure, hydraulic functions, and macropore flow, can be simulated with a new physico-empirical approach. The effects of tillage on the hydraulic properties are expressed through van Genuchten's α parameter, while empirical relationships are used to track changes in parameters related to soil structure (diffusion pathlength or effective aggregate size, kinematic exponent describing macropore tortuosity), as a function of cumulative rainfall following a tillage event.
4.) Kinetic sorption has been incorporated into the model, following the 'two-site' model approach described by Altfelder et al. (2000). This is applied only to the micropore region.

The updated version of MACRO (v5.0) requires six parameters in addition to those needed for a chromatographic model based on Richards equation and the convection-dispersion equation: the mixing depth, two additional hydraulic properties defining the boundary between macropores and micropores (water tension and hydraulic conductivity), the kinematic exponent, the macroporosity and the fraction of sorption sites equilibrating with macropore water.

One important reason why macropore flow models have not been widely adopted in exposure and risk assessments for agrochemical leaching is the difficulty of parameterization. Therefore, an automatic parameter calibration routine has been incorporated into the shell program for version 5.0 of MACRO. This inverse capability is supplied by the SUFI methodology described by Abbaspour et al. (1997). SUFI is a Bayesian global search algorithm that is considered well suited to complex simulation models such as MACRO, since it minimizes the risk of falling into local optima in the *n*-dimensional parameter space. The user first defines a prior uncertainty range or domain for each parameter to be estimated. This range is divided into a number of equal-size 'strata' and the first moment of each stratum defines the parameter estimate. All combinations of parameters are then run, and the value of a user-defined objective function (i.e. root mean square error or model efficiency, Loague and Green, 1991) is calculated for each simulation by comparing to measured data. Based on a critical tolerance for the objective function, the parameter ranges are refined (i.e. narrowed) for subsequent iterations by rejecting parameter values that perform badly. This kind of optimisation technique would have been too time-consuming for routine applications with earlier versions of the model, but the enhanced speed of execution of version 5.0 makes such methods more practicable.

In this paper, the existing FOCUS version of MACRO (4.3) and the new version (5.0) are compared to the results of the leaching experiment carried out in the structured clay soil at Lanna, Sweden (Larsson and Jarvis, 1999).

RESULTS AND DISCUSSION

The PELMO model

The pesticide input parameters used in the PELMO simulations are given in Table 1, while the calibrated values of the three preferential flow parameters are shown in Table 2. Figures 1 to 4 show a comparison of the measured concentrations in drainflow and in the soil profile, with the model simulations. The FOCUS version of PELMO failed to predict any leaching of the moderately strongly adsorbed compound imidacloprid at Andelst, while the new preferential flow version matched the timing and magnitude of the peak concentrations (c. 6 to 7 μg L^{-1}) measured in autumn drainflow, and also the subsequent decline in concentrations during the following winter (figure 1). According to the simulations, macropore flow only had a marginal impact on the resident concentrations in the profile, which were well matched by both model versions (figure 2). FOCUS PELMO did predict some leaching of the very weakly adsorbed herbicide bentazone at Lanna, although the initial breakthrough was delayed by c.100 days, and the concentrations and loads were seriously underestimated (figure 3). The preferential flow version of PELMO represented an improvement in that the overall level of the concentrations and loads better matched the data, but the dynamics of the leaching pattern at Lanna were poorly captured, indicating that the description of preferential flow and transport is perhaps too oversimplified in this case. Figure 4 shows that PELMO adequately matches the bentazone concentrations measured in the soil profile, and that the new macropore flow routine predicts slightly more leaching to depth, and less retention closer to the soil surface, although the differences are again small. The results for PELMO at Lanna can be compared to the performance of MACRO, which appears better able to describe the flow dynamics in this soil (Larsson and Jarvis, 1999, figure 5). One possible reason is the fine structure in the Lanna clay soil, especially in the subsoil, which means that the assumption in PELMO of direct transport from the surface to the base of the macropores (70 cm depth, Table 2) is unreasonable, whereas the coarser subsoil structure at Andelst better matches this assumption. Table 2 shows that although Lanna and Andelst have similar textures, the values of I_c and f derived by calibration imply that macropore flow is more pronounced and occurs more frequently at Lanna than at Andelst.

Table 1: Pesticide input data for the PELMO model

Parameter	Lanna (bentazone)	Andelst (imidacloprid)
Application date	18 October 1994	27 May, 1998
Application rate (kg ha^{-1})	2.508	0.7
DT50 (days)	12.5	336.5
T_{Ref} (°C)	20	10
Q10	2.2	2.9
K_{OC} (L kg^{-1})	5	127
Freundlich exponent	1.0	0.81

Table 2: Preferential flow parameters used for the PELMO simulations (calibrated).

Parameter	Lanna	Andelst
Depth of macropores (cm)	70	85
Threshold Rainfall, I_c (mm)	5	10
Fraction of excess rain routed into macropores, f	0.50	0.25

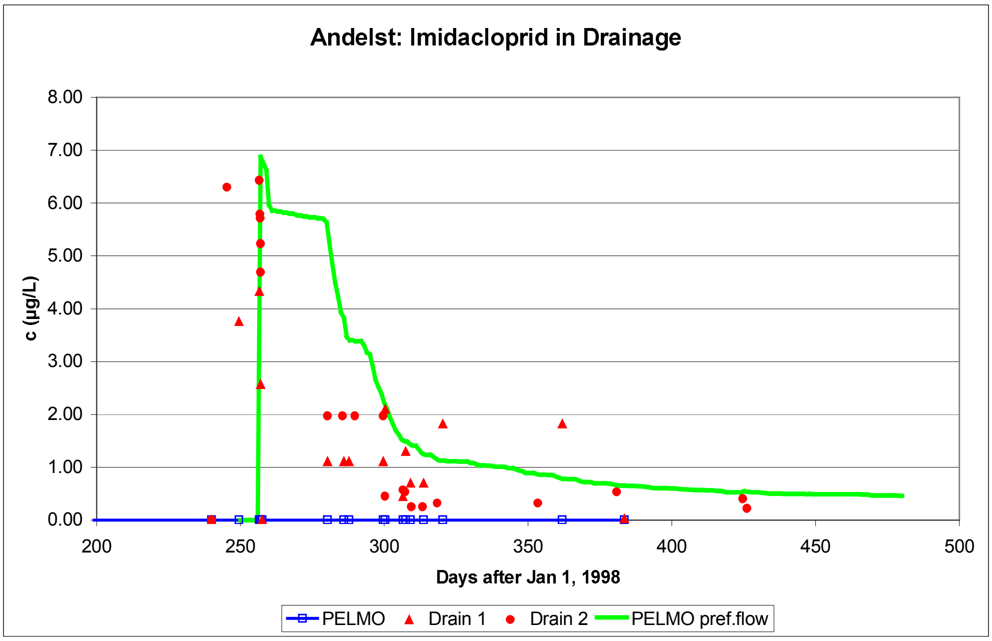

Figure 1: PELMO model simulations of imidacloprid concentrations in drainflow at Andelst

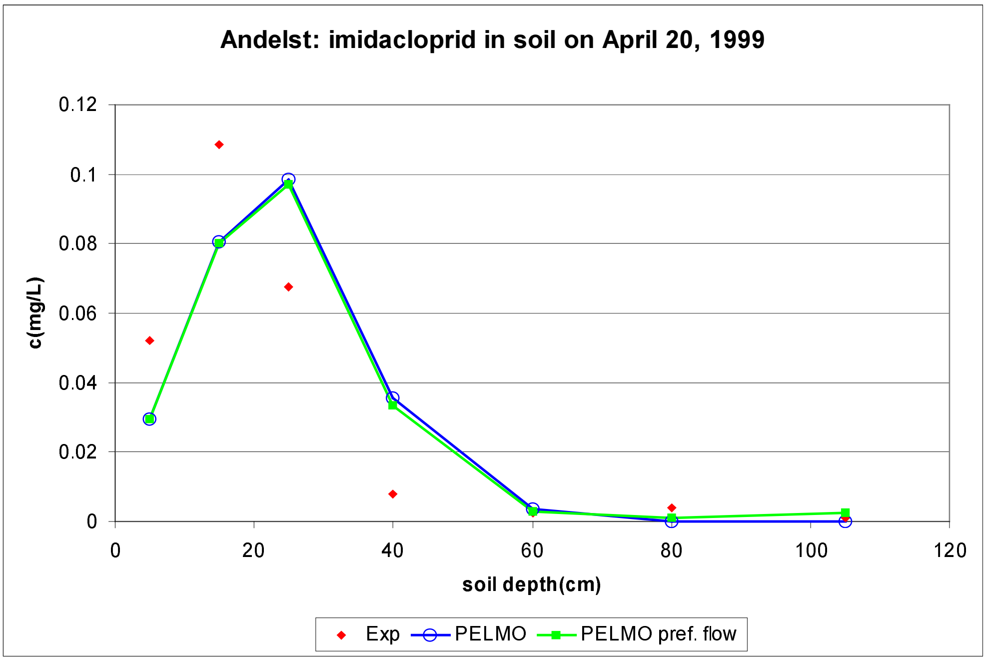

Figure 2: PELMO simulations and measurements of imidacloprid concentrations in soil

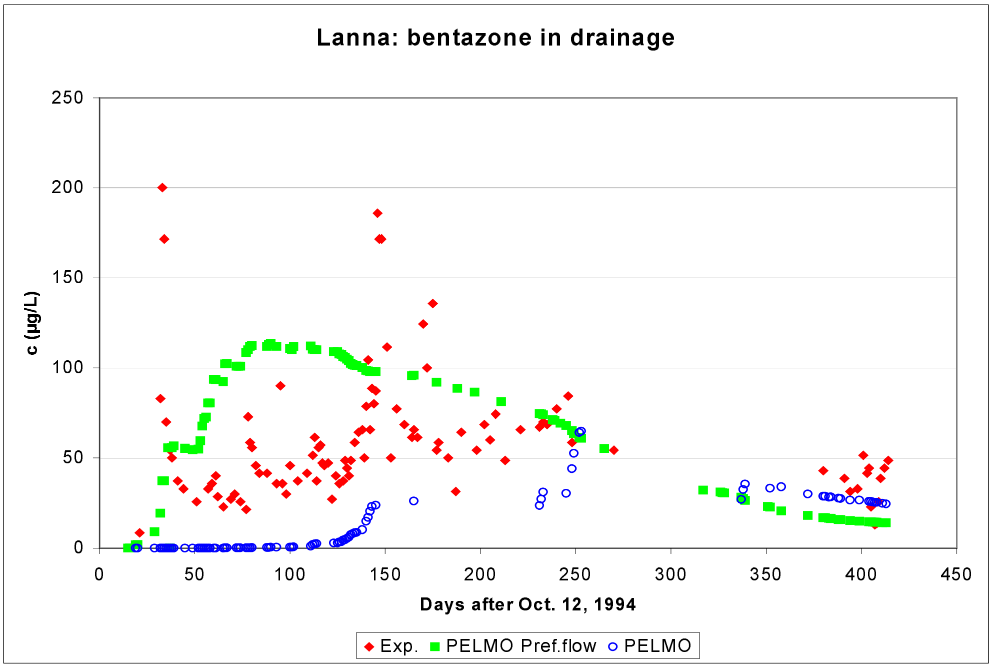

Figure 3: PELMO model simulations of bentazone concentrations in drainflow at Lanna

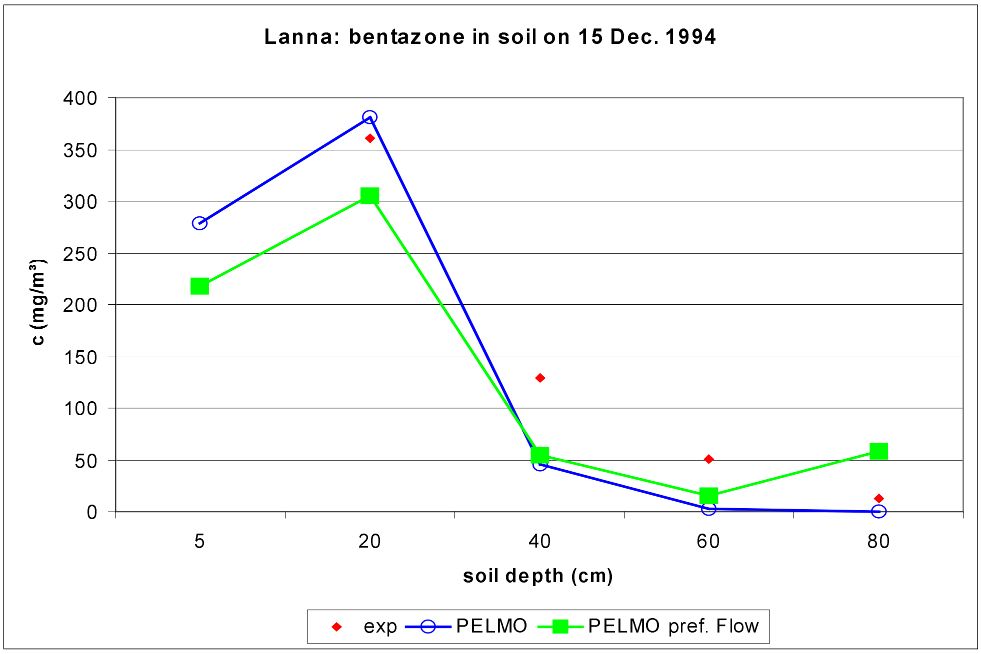

Figure 4: PELMO simulations and measurements of bentazone concentrations in soil

The MACRO model

Although the test results are not shown here, the change from Brooks-Corey to van Genuchten hydraulic properties makes little difference to predictions of water flow with MACRO providing the Brooks-Corey function gives a reasonable fit to the measured water retention data. However, such a good fit is not always guaranteed, especially for finer-textured soils (Scorza Junior, 2002). Therefore, the extra flexibility provided by the van Genuchten function represents a significant improvement in MACRO, but at the cost of one extra parameter.

One of the main advantages of the updated version of MACRO is speed; depending on the nature of the simulation, it runs c. 5 to 20 times faster than the previous version of the model. This makes the use of inverse techniques to estimate macropore flow parameters more practicable. Table 3 compares calculated model efficiencies for the various kinds of data available at Lanna for the two versions of MACRO, and in the case of MACRO5.0, for two different goal functions used in the optimization procedure.

Table 3. Model efficiencies calculated for all measured data points (Lanna).

	MACRO 4.3	MACRO 5.0	
Goal function in SUFI	Root mean square error	Root mean square error	Model efficiency
Soil moisture profiles	0.88	0.58	0.47
Bromide profiles	0.66	0.47	0.45
Bentazone profiles	0.90	0.58	0.79
Bromide concentration in drainage	0.37	0.33	0.69
Bentazone concentration in drainage	0.29	0.43	0.57
Drainflow	0.29	0.45	0.47

Table 4 Estimated parameter values (Lanna). Ranges indicate the posterior uncertainty domains (ASCALE = diffusion pathlength, mm; KSM = saturated matrix hydraulic conductivity, mm h^{-1}; RGWFLOW = Residence time, groundwater flow, days; DEG = degradation rate coefficient, $days^{-1}$ at 20°C).

Parameter	MACRO 4.3	MACRO 5.0	
	Root mean square error	Root mean square error	Model efficiency
ASCALE (0-30cm)	253 (223-400)	169 (141-313)	289 (235-300)
ASCALE (30-60cm)	61 (46-76)	357 (140-400)	203 (107-300)
ASCALE (60-100cm)	65 (44-86)	357 (226-400)	32 (10-203)
ASCALE (100-175cm)	31.5 (2-179)	350 (10-400)	117 (10-139)
KSM (0-1cm)	0.112 (0.1-0.172)	0.0765 (0.073-0.087)	0.067 (0.01-0.12)
RGWFLOW	4.5 (1-5.2)	33.8 (1-40.3)	40 (20-60)
K_{OC} cm^3 g^{-1}	4.84 (4.58-5.38)	3.11 (1-5.22)	2.17 (1.66-4.68)
DEG (0-30cm)	0.04 (0.03-0.046)	0.106 (0.07-0.113)	0.112 (0.11-0.14)
DEG (30-175cm)	0.01 (0.004-0.028)	0.0315 (0.003-0.06)	0.031 (0.025-0.048)

Table 3 shows that both versions of the model produce acceptable fits to the data, and that the new version does not perform better than the existing FOCUS version, at least for this dataset. The choice of goal function appears to be important when several data sources are combined into one overall measure of goodness of fit: the model performance can be significantly influenced (Table 3), and just as importantly, the best-fit parameter estimates may also change due to the optimisation methodology selected (Table 4). In principle, the model efficiency should be preferred, since it has the advantage of the numerical value being independent of the units of the data source. Nevertheless, the differences in parameter estimates between different model versions seem to overshadow the effects of different optimisation methods: version 5 predicts much longer residence times of local shallow lateral groundwater flow (values which seem much more reasonable given the size of the plots, 0.4 ha), slightly weaker sorption and considerably larger degradation rate coefficients in both topsoil and subsoil. Table 4 also shows that one important parameter regulating the strength of macropore flow (the diffusion pathlength) could only be identified within very wide posterior uncertainty bounds, especially in the topsoil, and deeper subsoil, and for the new version of the model. The reason for this is not clear, but it may be related to the simplified first-order description of mass exchange between the flow domains, which fails to capture the short-term fluctuations observed in drainflow concentrations (fig.5).

CONCLUSIONS

The new description of macropore flow incorporated into the FOCUS PEC model PELMO appears promising, and in the preliminary tests presented here gave significantly improved predictions of leaching in two structured clay soils. Additional testing against more field data would help to gain further understanding of how this empirical approach should be parameterized, and whether the parameters in the model can be related to measurable soil physical quantities (e.g. clay content).
The new version of MACRO (5.0) represents a considerable improvement compared to the currently available version of the model, partly in terms of improvements to process descriptions (e.g. tillage, kinetic sorption) and numerical accuracy, but also with respect to useability. The model runs in a Windows environment, at a much faster speed, which in turn enables advanced, automated, methods for parameter estimation. However, more research is needed to identify the data requirements for reliable inverse estimation of model parameters related to macropore flow.

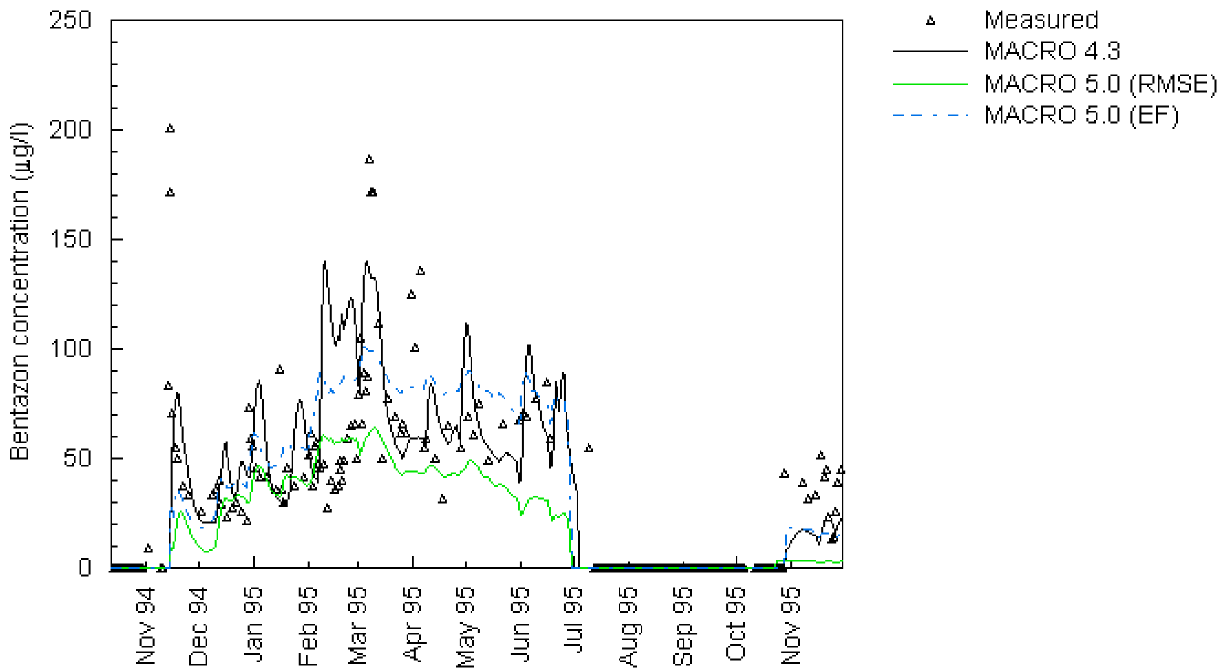

Figure 5: Bentazone concentrations in drainflow at Lanna simulated with MACRO

ACKNOWLEDGEMENTS

This work was funded in the 5th framework project APECOP ('Effective approaches for assessing the predicted environmental concentrations of pesticides', contract no. QLK4-CT-1999-01238).

REFERENCES

Abbaspour, K.C., van Genuchten, M.T., Schulin, R., Schläppi, E., 1997. A sequential uncertainty domain inverse procedure for estimating subsurface flow and transport parameters. Water Resources Research, 33: 1879-1892.

Altfelder, S., Streck, T., Richter, J. 2000. Nonsingular sorption of organic compounds in soil: the role of slow kinetics. Journal of Environmental Quality, 29: 917-925.

Beven, K., Germann, P., 1982. Macropores and water flow in soils. Water Resources Research, 18: 1311-1325.

FOCUS. 2000. FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference SANCO/321/2000 rev.2, 202pp.

FOCUS. 2001. FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC. Report of the FOCUS Working Group on Surface Water Scenarios, EC Document Reference SANCO/4802/2001-rev.1. 221 pp.

Germann, P. 1985. Kinematic wave approach to infiltration and drainage into and from soil macropores. Transactions of the ASAE, 28: 745-749.

Hendrickx, J.M.H., Dekker, L.W., Boersma, O.H. 1993. Unstable wetting fronts in water repellent field soils Journal of Environmental Quality, 22: 109-118.

Hendriks, R.F.A., Oostindie, K., Hamminga, P. 1999. Simulation of bromide tracer and nitrogen transport in a cracked clay soil with the FLOCR/ANIMO model combination. Journal of Hydrology, 215: 94-115.

Jarvis, N.J., 1994. The MACRO model (Version 3.1) - Technical description and sample simulations. Reports and Dissertations, 19, Dept. Soil Sciences, Swedish Univ. Agric. Sciences, Uppsala, Sweden, 51 pp.

Jarvis, N.J., 2002. Macropore and preferential flow. In: The Encyclopedia of Agrochemicals, (ed. J. Plimmer), vol.3, 1005-1013, J. Wiley & Sons, Inc.

Klein, M., 1995. PELMO: Pesticide Leaching Model, User manual version 2.01. Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, Schmallenberg.

Larsson, M.H., Jarvis, N.J., 1999. Evaluation of a dual-porosity model to predict field-scale solute transport in macroporous soil. Journal of Hydrology, 215: 153-171.

Loague, K.M., Green, R.E. 1991. Statistical and graphical methods for evaluating solute transport models: overview and application. Journal of Contaminant Hydrology, 7: 51-73.

Roth, K., 1995. Steady-state flow in an unsaturated, two-dimensional, macroscopically homogeneous, Miller-similar medium. Water Resources Research, 31: 2127-2140.

Scorza Junior, R. 2002. Pesticide leaching in macroporous clay soils: field experiment and modeling. PhD thesis, Wageningen University, The Netherlands.

van Dam, J. 2000. Field-scale water flow and solute transport : SWAP model concepts, parameter estimation and case studies. PhD thesis, Wageningen University, The Netherlands.

Van Genuchten, M.T. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Science Society of America Journal, 44: 892-898.