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FOOTPRINT

Functional Tools for Pesticide Risk Assessment and Management

Specific Targeted Research Project

Thematic Priority: Policy-orientated research

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Algorithm to completely parameterise MACRO from basic soil property data and soil and crop management options

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PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

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Foreword

The present report was prepared within the context of the work package WP4 ('Model parameterisation, meta-modelling and risk assessment') of the FOOTPRINT project (www.eu-footprint.org). The document integrates deliverables 19 and 21 which both deal with the parameterisation of the pesticide leaching model MACRO.

The preferred reference to the present document is as follows:
Jarvis N., Lindahl, A., Messing, I., Stenemo, F., Hollis, J., Reichenberger, S. & Dubus, I.G. (2007). Algorithm to completely parameterise MACRO from basic soil property data. Report DL21 of the FP6 EU-funded FOOTPRINT project [www.eu-footprint.org], 18p.

Executive summary

MACRO is a one-dimensional dual-permeability model that can account for the effects of macropore flow on leaching. MACRO will be used in the EU project FOOTPRINT to make EU-wide predictions of pesticide leaching to groundwater and to surface waters via sub-surface drainage systems. This presents considerable challenges in terms of model parameterization, since most parameters are not directly available, and must therefore be derived from specific parameter estimation algorithms ('pedotransfer functions'). In the following, we describe the underlying hydro-pedological concepts and specific pedotransfer functions that will be used in FOOTPRINT to estimate i.) the soil hydraulic functions, focusing especially on the model parameters controlling macropore flow, and ii.) the bottom boundary condition in the model, which largely controls the site hydrology, and especially the partitioning of excess water between groundwater recharge and discharge to surface waters.

Several data sources are used to support the calculation of model parameters: the Soil Geographic Database of Europe, v. 1.0 was used to identify 249 'benchmark' soil profiles ('FOOTPRINT soil types') that characterise agricultural land in Europe. The following data, which is available in the SPADE-2 database for each soil horizon, is used to support the parameterization of hydraulic properties in the model: horizon designation; upper depth (cm); lower depth (cm); clay, silt and sand (%); stone content (%); pH; organic carbon content (%); bulk density (g cm^{-3}). Each soil type is classified into one of eight unique hydrological classes based on the HOST ('Hydrology of Soil Types') system. This defines the bottom boundary condition in MACRO and is also used to support the definition of drainage systems for those sites that are subsurface drained.

1 INTRODUCTION

This report presents the results of work carried out within the FOOTPRINT project to develop a consistent and complete set of parameter estimation routines for the pesticide leaching model MACRO (Larsbo and Jarvis, 2003) that enable EU-wide simulations of pesticide leaching based on only readily available data (e.g. soil survey data and soil profile descriptions). This report focuses especially on algorithms developed to meet two major challenges in this respect, namely parameter estimation routines that account for the effects of soil structure/morphology and site hydrological conditions on pesticide losses to surface waters and groundwater. The parameterisation system developed in the FOOTPRINT project shares the same underlying philosophy as the earlier software package MACRO-DB (Jarvis et al., 1997). Existing estimation routines have been upgraded and improved to reflect advances in process understanding and the more extensive empirical support available today, and some new functions have been developed. The system is compatible with the data available at the EU level, and that which farmers and extension advisors could gather quickly and at reasonable cost at the local field and farm scales.

2 METHODS

The algorithms described in this section are used in FOOTPRINT to parameterize MACRO for EU-wide predictions, as a basis for 'look-up' tables (i.e. the meta-model approach). Some additional routines will be available in the 'stand-alone' (real-time simulations) version of MACRO that will also be available to users of the FOOT tools. These additional routines will allow users to simulate the effects of a wider range of processes and management options, such as pH effects on sorption of acids, no-till soil management, different pesticide application methods, and soil compaction.

2.1 Soil hydraulic parameters

2.1.1 Soil water retention

MACRO uses the van Genuchten (1980) water retention equation. The parameters of this soil water retention function (the shape parameters α, n, and the nominal saturated water content θ_s, assuming that $m = 1-1/n$ and the residual water content θ_r is zero) are estimated from basic soil properties (e.g. texture, bulk density, organic carbon content) using the HYPRES continuous pedotransfer functions (Wösten et al., 1999). Water retention parameters for organic horizons are set to fixed values ($\alpha = 0.013$ cm^{-1} and $n = 1.2$) based on measured data for 148 organic soil horizons in Europe (Wösten et al., 1999).

The nominal saturated water content θ_s predicted by HYPRES is corrected for stone content by multiplying by the factor $1-(f_s(1 - \varepsilon_s))$ where f_s is the volumetric stone content and ε_s is the stone porosity, which is assumed to be 0.1 for FOOTPRINT substrate geologies D, E and F and zero for all others.

In a review of the literature, Jarvis (2007) concluded that the weight of empirical evidence suggests that pores of ‘equivalent cylindrical diameter’ larger than about 0.3 mm can be considered as macropores. Thus, the minimum water potential defining the boundary between macropores and matrix in MACRO (parameter CTEN) is fixed at -10 cm, and the saturated matrix water content (i.e. XMPOR, the water content at -10 cm, θ_{10}) is estimated from the van Genuchten parameters. In this respect, it should be noted that the saturated water content θ_s calculated by HYPRES is only used to calculate the saturated matrix water content, θ_{10}, and is not actually used as a parameter in the model, since macroporosity (and thus total saturated water content) are estimated independently (see section 2.1.2).

The wilting point water content (WILT) is estimated from the van Genuchten parameters as the water content at a tension of 150 m.

2.1.2 Soil structure

Parameters controlling the strength of macropore flow in the model are estimated by class pedotransfer functions, since the experimental data were deemed insufficient to support the development of robust continuous functions. In our proposed approach, each horizon in the soil profile is placed into one of four classes with respect to the potential for non-equilibrium flow in macropores (see Figure 1), ranging from ‘no potential’ (class I) to high potential (class IV). The classification scheme is based on the idea that macropore flow is potentially strongest in soils characterised by a poorly developed ‘structure hierarchy’ (i.e. a soil in which the structural porosity is dominated either by coarse, strongly developed aggregates or large continuous biopores). Since soil structure descriptions are not available for the FOOTPRINT soil types, the scheme in Figure 1 predicts the strength of macropore flow from basic soil properties, land use and management practices, based on work relating aggregation and the abundance of earthworms to site and soil factors (Lindahl et al., in preparation).

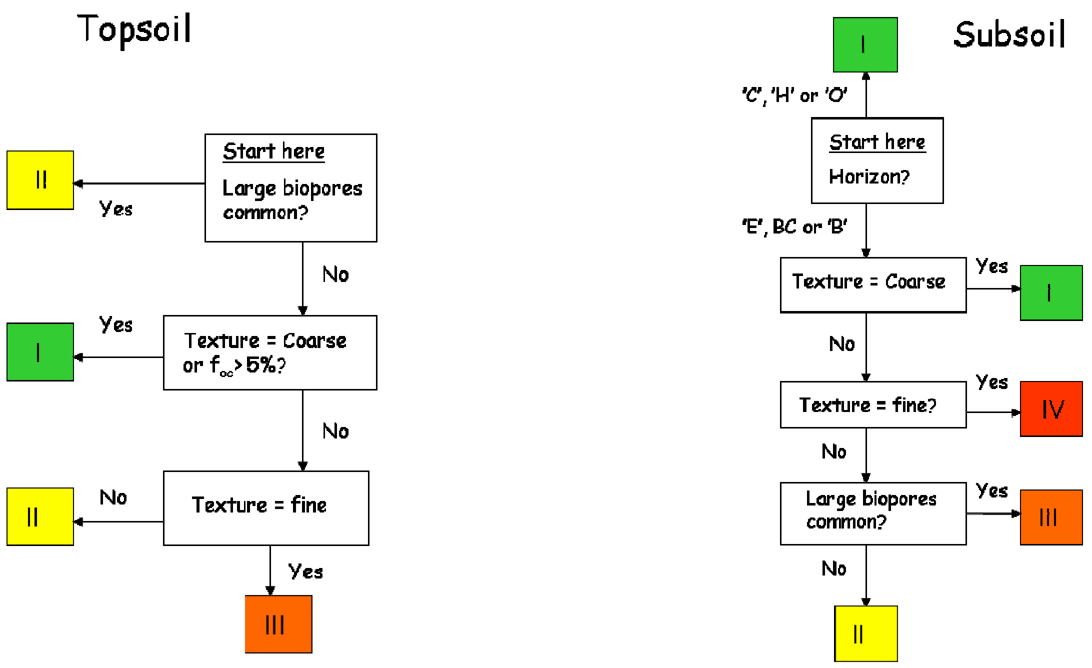

Figure 1. Decision-tree to classify soil horizons with respect to the strength of macropore flow. I = no potential, II = low potential, III = moderate potential, IV = high potential. Letters denote FAO (1990) horizon designations. Coarse texture = sand or loamy sand (USDA), fine texture = clay, silty clay or silty clay loam USDA). f_{oc} = organic carbon content.

Site factors			[d]Limiting soil texture
[a]Climate zone	[b]Hydrologic conditions	[c]Land use and management	
Cold temperate (FCZ 4,6,12,13,15)	All	Perennial	Coarse
Humid temperate (all other, except FCZ 10)	All	Perennial Annual	Coarse Coarse or fine
Mediterranean (FCZ 1,8,9)	Irrigated or FHC ≠ L,M or N	Perennial Annual	Coarse Coarse or fine

Table 1. Favourable site factors and soil textures limiting anecic earthworms.
[a]FCZ = FOOTPRINT climate zone; [b]FHC = FOOTPRINT hydrologic class (see section 2.3); [c]Perennial = grassland, orchards, vines, olives; [d]Coarse = sand/loamy sand, fine = clay/silty clay/silty clay loam

The scheme shown in Figure 1 considers the influence of large biopores (defined as cylindrical pores >2 mm in diameter, equivalent to medium, coarse, and very coarse biopores according to FAO, 1990) on the potential for macropore flow. Permanent channels created by anecic earthworms are considered here as the dominant factor affecting macropore flow (large root channels are ignored). Several studies show a good correlation between the numbers of live earthworms, burrow numbers and hydraulic properties. There is considerably more literature on earthworm populations than burrow densities, especially for a few well-studied species like *Lumbricus terrestris* L. The biopore algorithm is therefore based on a literature meta-analysis of factors controlling population densities of *Lumbricus terrestris* (Lindahl et al., in preparation) that includes measurements from 86 different sites in Europe. The simple algorithm described below correctly classified 79% of these studies.

Table 1 shows the combinations of site and soil factors that give favourable conditions for *Lumbricus terrestris*, defined as a population density greater than 8 m^{-2} (ca. 2 adult worms per m^2). Table 1 is combined with some simple rules to define one or more horizons in each FOOTPRINT soil type, that together comprise a zone in the soil profile which contains functional burrows, with respect to water flow and solute transport. The upper and lower limits, L_u and L_l, of the functional burrow zone are given by:

L_u = max(0, tillage depth)
L_l = upper boundary of first horizon with *limiting factor*

where *limiting factors* are one or more of the following: rock ('R'); drainage depth (see section 2.3.); 'BC', 'C' or 'O' horizon; pH<5; bulk density >1.75 g cm^{-3}; limiting texture (see Table 1).

Large functional biopores formed by anecic earthworms are then assumed to be common in a horizon (see Figure 1) if:

(mid-point depth of horizon > L_u*) and*
(mid-point depth of horizon < L_l*) and*
(site conditions are potentially favourable, see Table 1) and
(L_l *minus* L_u *> 20 cm)*

Two parameters in MACRO are directly estimated from the macropore flow classes (the effective diffusion pathlength ASCALE, and the kinematic exponent ZN, see Table 2) and one indirectly (saturated hydraulic conductivity, KSATMIN, see section 2.1.3).

Class	[a]Effective diffusion pathlength (mm)	Kinematic exponent
I	1	6
II	15	4
III	50	3
IV	150	2

Table 2. Class pedotransfer functions for soil structure-related parameters.
[a]the effective diffusion pathlength is set to 3 mm in the uppermost intensively tilled layer in arable soil independent of class. Intensive tillage (e.g. harrowing, rotovating) shatters and pulverizes the soil to create a fine 'crumb' or granular structure, with a spherical geometry that maximises mass exchange

No suitable estimation routines were available to estimate soil macroporosity. Nevertheless, a review of the literature carried out within FOOTPRINT suggests that, as a structure-related parameter, macroporosity is closely related to observable horizon morphology and basic soil properties such as texture (Jarvis, 2007). Therefore, macroporosity is estimated as a function of the FAO (1990) horizon designation and the soil texture (see Table 3). The total porosity (TPORV) is then simply given by the sum of macroporosity and θ_{10}.

Soil	Horizon	[a]Texture		
		Fine	Medium	Coarse
Topsoil (mineral)	[b]Undisturbed	0.05		
	[c]'A_t'	0.05		
	[d]'A_p'	0.03	0.04	0.05
Subsoil (mineral)	[e]Upper 'B' or 'E'	0.016	0.016	0.05
	[f]Lower 'B' or 'E'	0.008	0.008	0.05
	'BC'	0.002	0.004	0.04
	'C'	0.002	0.004	0.03
Organic	'O'	0.05		

Table 3. Class pedotransfer function for macroporosity.
[a]fine=clay,silty clay,silty clay loam, coarse = sand, loamy sand, medium = all others; [b]perennial crops i.e. grassland, vines, orchards, olives; [c]intensively (secondary) tilled uppermost soil layer; [d]ploughed but not secondary tilled; [e]mid-point depth of horizon <50 cm; [f]mid-point depth of horizon >50 cm

2.1.3 Hydraulic conductivity

Jarvis et al. (2002) showed that hydraulic conductivity at -10 cm, K_{10} (KSM) measured by tension infiltrometer was reasonably well predicted by soil texture. However, a more physically-based approach predicting K_{10} from the pore size distribution (i.e. van Genuchten water retention parameters) would be preferable. From a strictly physical point of view, K_{10} should depend only on α and θ_{10} when m = 1-1/n and θ_r is zero (Mishra and Parker, 1990; Hoffman-Riem et al., 1999). We re-analysed the data presented by Jarvis et al., (2002) using this physically-based model, but the results were poor. This is presumably because the van Genuchten parameters were not available for this dataset, and so they were predicted using the HYPRES pedotransfer functions. In particular, α is poorly estimated by the HYPRES function (Wösten et al., 1999). We therefore developed a physico-empirical approach using n as a predictor variable (Wise et al., 1994):

$$K_{10} = C\theta_{10}n^{l} \qquad (1)$$

where C and l are constants. Figure 2 compares measured and predicted K_{10} values with C = 0.186 mm h^{-1} and l = 10.73. The agreement must be considered satisfactory, considering the errors involved in predicting n and also the errors involved in the measurement of K_{10}, not least because they were performed by ten different researchers (Jarvis et al., 2002). This is illustrated by the fact that the measurements from three of the researchers fall consistently below the 1:1 line (Figure 2). Clearly, considering how it was derived, equation (1) should only be used to predict K_{10} in conjunction with the HYPRES pedotransfer functions, and not from measured water retention data.

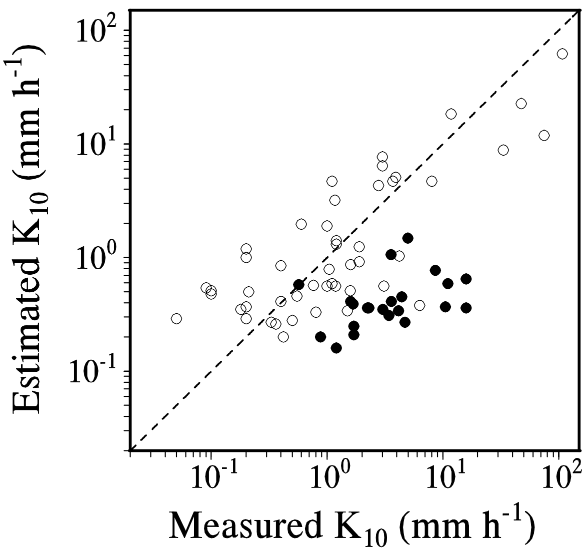

Figure 2. Measured and predicted saturated matrix hydraulic conductivity.
Data are taken from Jarvis et al. (2002), predicted values are calculated using equation 1, and θ_{10} and n are predicted by HYPRES. Solid symbols represent data obtained by three of the ten researchers.

If it is assumed that the macropore size distribution follows a power law function (i.e. a water retention curve of the Brooks-Corey type) and flow is calculated according to a capillary bundle model based on Poiseuille's law with a fixed maximum pore size, then the macropore saturated conductivity $K_{s(ma)}$ is given by (Jarvis, in preparation):

$$K_{s(ma)} = \frac{B\varepsilon_{ma}}{n^*} \qquad (2)$$

where ε_{ma} is the macroporosity (see Table 3), n^* is the kinematic exponent (ZN, see Table 2) and B is composite 'matching factor' accounting for both physical constants and the geometric irregularity of the functional macropore system, set here to 6000 mm h^{-1}. The total saturated hydraulic conductivity (KSATMIN) is simply given by $K_{10} + K_{s(ma)}$.

2.2 Rock hydraulic parameters

One FOOTPRINT hydrologic class represents free-draining soils overlying permeable rock, where recharge to groundwater is the dominant flow pathway (i.e. classes L, M, and N, see section 2.3). In some FOOTPRINT soil types the boundary between soil and rock occurs at relatively shallow depths (e.g. thin 'rendzina' soils overlying chalk). In these situations, MACRO must be run to a profile depth of 2 m (i.e. well into the rock layer) to ensure that a reasonable hydrology is simulated with the bottom boundary condition used (unit hydraulic gradient, see section 2.3). This means that hydraulic properties must be defined for the permeable rock. Soil hydrologic groups L, M and N overly substrate geologies D, E, and F, which mostly represent rocks such as fissured chalk, limestone and sandstone. For this special case of permeable rock horizons, we set the hydraulic parameters in MACRO to values that represent fissured limestone (Roulier et al., 2006), assuming a high potential for macropore flow (i.e. class IV): effective diffusion pathlength = 150 mm; $K_{s(ma)}$ = 30 mm h^{-1}; K_{10} = 0.04 mm h^{-1}; θ_s = 0.1 m^3 m^{-3}; α = 0.0004 cm^{-1}; n = 1.8; n^* = 2; ε_{ma} = 0.01 m^3 m^{-3}.

2.3 Site hydrology

Using the HOST methodology (Boorman et al., 1995), each FOOTPRINT soil type has been classified into one of 14 hydrologic classes (L to Y), on the basis of the major pathways of water flow and pesticide loss in the profile. These hydrologic classes then form the basis of the parameterisation of surface runoff in PRZM and also affect parameters controlling drainage and leaching in MACRO, specifically the bottom boundary condition and the dimensions of any drainage system present. For MACRO, the 14 classes can be telescoped further into 8 unique hydrologic parameterisations (see Table 4). Three major groupings are recognised: classes L,M and N represent soils with free drainage to deep-lying groundwater. A unit hydraulic gradient bottom boundary condition is used, no drains are present, all excess water is routed to groundwater, and only pesticide leaching is output from the model (Table 4). Another group (W, X and Y) represents soils with slowly permeable substrate, that allow both recharge to groundwater and discharge to surface waters (via subsurface drains and/or lateral subsurface flow). A water table is found within the profile depth, and the bottom boundary condition is given by a percolation rate defined as a linear function of the water table height. Only discharge to surface water is simulated for the third group of soils, which either have impermeable substrates (i.e. hard rock or impervious clay, classes R to V) or are located in low-lying areas in the landscape (O to Q). The bottom boundary condition is, thus, zero flow and discharge is simulated via subsurface drains.

Hydrologic class	Drainage depth (m)	Depth of profile (m)	Bottom boundary condition	MACRO output variables
L,M,N	N/A	2	Unit hydraulic gradient	Percolation rate Leaching rate
O,P	2	2	Zero flow	Drainage rate Loss in drain Conc. at base
Q	1	2	Zero flow	Drainage rate Loss in drains Conc. at base
R,S,T	[a]Calculated	[c]Calculated	Zero flow	Drainage rate Loss in drains
U,V	[b]Calculated	[c]Calculated	Zero flow	Drainage rate Loss in drains
W	[a]Calculated	2	Percolation rate regulated by water table height	Percolation rate Leaching rate Drainage rate Loss in drains
X	[a]Calculated	2	Percolation rate regulated by water table height	Percolation rate Leaching rate Drainage rate Loss in drains
Y	[b]Calculated	2	Percolation rate regulated by water table height	Percolation rate Leaching rate Drainage rate Loss in drains

Table 4. Hydrologic classes as a basis for MACRO parameterisation.
[a] minimum of: i.) depth to rock, ii.) profile depth
[b] minimum of: i.) depth to rock, ii.) depth to 'C' horizon, if texture= fine/medium iii.) 1 m
[c] minimum of: i.) depth to rock, or ii.) 2 m

An 'effective' drainage spacing, *L* (SPACE), is calculated for each soil type belonging to one of the FOOTPRINT hydrological classes which include discharge to surface water (classes O to Y), following the methodology introduced by Hooghoudt (1941):

$$L = \sqrt{\frac{8K_2 dh + 4K_1 h^2}{q_{eff}}} \qquad (3)$$

$$d = \frac{D}{\left(\frac{8D}{\pi L}\right)\ln\left(\frac{D}{u}\right) + 1} \qquad (4)$$

where d is a reduced 'effective' soil depth below the drainage base, q_{eff} is a design discharge rate, h is the design height of the water table above the drainage base, D is the actual depth of soil between the drainage depth (DRAINDEP) and the bottom of the profile (see Table 4), K_1 and K_2 are the weighted average saturated hydraulic conductivities (KSATMIN) across the soil depths h and D respectively, and u is the wetted perimeter of the drainage channel. It can be noted from equations 3 and 4 that L depends on d and d on L. The drain spacing L is therefore found iteratively when $D>0$.

L is an 'effective' drainage spacing: some FOOTPRINT hydrologic classes typically have field drains installed (e.g. parallel pipe or tile lines), while others would instead be drained by open ditches surrounding the field. Finally, in some classes (i.e. R, S, T, W and X), an 'effective' drainage system is simulated to mimic lateral downslope saturated flow above an impermeable substrate towards ditches and streams. In the absence of parallel field drains, the 'drain spacing', *L*, can be related to the effective area of a square-shaped drainage basin (Larsbo and Jarvis, 2003).

The wetted perimeter of the drainage channel, which is unknown, is fixed at 0.2 m, although it could in reality vary between ca. 0.1 and 0.5 m depending on the type of drainage system.

The design water table height, *h*, is set to the drainage depth, or to 0.7 m, whichever is the smallest. In other words, for poorly drained sites, we assume that to achieve sustainability in agricultural systems (at least for those in which pesticides would typically be used), the drainage system (either natural or artificial) must be sufficient to prevent the water table from rising to the soil surface at the design discharge rate.

The design discharge is calculated as:

$$q_{eff} = P - q_{out} \tag{5}$$

where P is a design recharge rate and q_{out} is an average percolation rate at the base of the profile during the same period. The percolation rate q_{out} is obviously fixed at zero for the FOOTPRINT hydrological classes with zero flow as the bottom boundary condition, but it takes a positive value for the class with slowly permeable substrate (W, X and Y): given the bottom boundary condition employed in MACRO for this hydrologic group, q_{out} can be expressed as a linear function of the average water table height above the base of the soil profile, under natural drainage conditions (i.e. in the absence of artificial drains) H:

$$q_{out} = B_{grad} H \tag{6}$$

where B_{grad} is the parameter (time constant) in the MACRO model (BGRAD) that controls percolation to groundwater. In FOOTPRINT, B_{grad} is estimated as:

$$B_{grad} = \frac{p_{gw} R}{H} \tag{7}$$

where R is the percolation rate (excess of precipitation over actual evapotranspiration) during the field capacity period and p_{gw} is the proportion of the excess water that percolates to groundwater. Thus, equation 5 can be re-written as:

$$q_{eff} = P - p_{gw} R \tag{8}$$

The parameter R obviously depends on climate and has been estimated for each of the FOOTPRINT climate zones by simple water balance modelling. The parameters p_{gw} and H are set in FOOTPRINT to reflect the original conceptual models underlying the HOST hydrologic classification system. For the sake of simplicity, p_{gw} and H are set to 0.5 and 0.5m respectively for hydrologic class W, and to 0.25 and 1.5m for classes X and Y. This implies that, in the same climate zone, B_{grad} is 6 times larger for class W than for X and Y. Table 5 shows the values of R and resulting values of B_{grad} (BGRAD) for each climate zone.

P should reflect a typical maximum amount of water recharging the water table on any day, and will therefore depend strongly on the depth of the water table in the soil (short-term peak flows in surface soil are 'damped out' with depth). Therefore, in FOOTPRINT, *P* is set to:

$$P = \max(R,\ \max(20,\ 30 - 20z)) \tag{9}$$

where z is the depth of the drainage base below the soil surface (in metres) and P and R are given in units of mm day^{-1}. This simple expression implies that *P* goes from a maximum of 20 mm day^{-1} for shallow lateral flow (i.e. drain depth of 0.5 m depth or less) to a minimum value equivalent to *R* if the drainage base is much deeper than 1 m.

FCZ	R (mm/day)	BGRAD	
		Class W	Class X and Y
1	1.93	8.0E-05	1.3E-05
2	1.47	6.1E-05	1.0E-05
3	2.38	9.9E-05	1.7E-05
4	1.14	4.8E-05	7.9E-06
6	6.55	2.7E-04	4.5E-05
7	2.58	1.1E-04	1.8E-05
8	2.64	1.1E-04	1.8E-05
9	2.98	1.2E-04	2.1E-05
10	1.25	5.2E-05	8.7E-06
11	2.94	1.2E-04	2.0E-05
12	5.93	2.5E-04	4.1E-05
13	5.93	2.5E-04	4.1E-05
14	1.23	5.1E-05	8.5E-06
15	0.99	4.1E-05	6.9E-06
16	1.91	8.0E-05	1.3E-05

Table 5. Estimated values of *R* and BGRAD (1/hour) for slowly permeable substrates.

2.4 Crop parameters

Crop parameters in MACRO (Tables 6, 7 and 8) are set partly according to FOCUS (2001) and partly based on information on drought tolerance and root depths in Allen et al. (1998). It should be noted that the maximum root depth shown in Tables 6 and 7 is reduced in the presence of a limiting soil horizon, following the decision rules in MACRO_DB (Jarvis et al., 1997). A horizon is considered limiting to root penetration if:

('C' or 'R' horizon) or
(pH $\leq$ 4.5) or
((sand content (%)> 85- (silt content (%). 0.5)) and $f_{oc} \leq 0.2\%$) or
$f_{st} > 0.2$ or
('subsoil' and 'structure class = I') and (bulk density > 1.65 g cm^{-3})

Parameter	Crop grouping								
	A	B	C	D	E	F	G	H	I
Maximum leaf area index (LAIMAX)	5	5	4	4	3	5	5	5	4
Green leaf area index at harvest (LAIHARV)	1	5	2	3	3	2	0.01	3	4
[a]Drought tolerance	Medium	Medium	Low	Medium	Low	Medium	Medium	High	Medium
Maximum root depth (m) (ROOTMAX)	1.1	0.8	0.5	0.8	0.5	1.1	1.4	1.1	0.8
Max. Interception capacity (mm) (CANCAP)	2	2	2	2	2	3	3	2	2
Ratio evaporation of intercepted water to transpiration (ZALP)	1.0	1.0	1.0	1.0	1.0	1.5	1.5	1.0	1.0

Table 6. MACRO annual crop parameters.
A: Soft wheat, barley, rye, durum wheat, oats, flax, oilseed, rapeseed; B: Sugar beet, fodder root; C: Potato; D:Soya, pulses; E: Fresh vegetables; F: Maize grain, fodder maize, sunflower; G: Vineyards, orchards in all FCZ's except 8 and 9; H: Cotton; I: Tobacco. [a] transpiration adaptability factor (BETA): low = 0.5, medium = 0.2, high = 0.1; critical tension for transpiration reduction (WATEN) is calculated from the known soil properties together with the % of extractable micropore water exhausted before reduction in transpiration occurs: low = 50%, medium = 65%, high = 80%

Parameter	Crop grouping		
	Grassland/ green fodder	Orchard (FCZ 8,9)	Olives
Leaf area index (LAIC)	5	5	3
[a]Drought tolerance	Medium	Medium	High
Root depth (m) (ROOTDEP)	0.8	1.4	1.4
Max. Interception capacity (mm) (CANCAP)	2	2	1
Ratio evaporation of intercepted water to transpiration (ZALP)	1.0	2.0	2.0

Table 7. MACRO perennial crop parameters.
[a] transpiration adaptability factor (BETA): low=0.5, medium=0.2, high=0.1; critical tension for transpiration reduction (WATEN) calculated from known soil properties and the % of available water exhausted before reduction in transpiration occurs: low=50%, medium=65%, high=80%

Parameter	Value
Root distribution (RPIN)	67%
Leaf development factor, growth (CFORM)	1.6
Leaf development factor, senescence (DFORM)	0.3
Leaf area index on specified day[a] (LAIMIN)	0.01
Root depth on ZDATEMIN[a] (m) (ROOTINIT)	0.01
Critical air content for transpiration reduction (m^3 m^{-3}) (CRITAIR)	0.05

Table 8. MACRO parameters constant for all crops.
[a] for spring-sown arable crops. For autumn-sown arable crops, LAIMIN and ROOTINIT are set to 1.0 and 0.2 respectively. For crop group G, ROOTINIT is set to 95% of the maximum root depth.

2.5 Solute transport

Apart from the diffusion pathlength (see section 2.1), all solute transport parameters are set to fixed values: the diffusion coefficient (DIFF) is set to the default value in FOCUS, namely 5 x 10^{-10} m^2 s^{-1}, the fraction of sorption sites in the macropores (FRACMAC) is set to 0.01, the mixing depth (ZMIX) is set to 1 mm and the anion exclusion water content (AEXC) to zero. In MACRO, the solute dispersivity (DV) is required to simulate dispersion in the soil matrix using the advection-dispersion equation. A few pedotransfer functions have been developed, but these have been based on experiments carried out on saturated soil (Goncalves et al., 2001; Perfect et al., 2002) where macropores tend to dominate the observed dispersion. It would clearly not be appropriate to use such functions in conjunction with MACRO. Vanderborght and Vereecken (2007) recently described a database of dispersivities consisting of 635 values abstracted from 57 published studies. They showed that dispersivity tended to increase with the scale of the leaching experiment (from core to column to field), with flow rate, and with the distance travelled. An examination of a subset of the data presented by Vanderborght and Vereecken (2007) suggests that these effects are primarily due to preferential flow: we selected only those data (n = 116) obtained from experiments carried out at steady flow rates of less than 1 mm h^{-1}, since macropore flow could then reasonably be excluded (it should be noted that the subset analysed only contained experiments carried out on five texture classes with relatively small clay contents and, presumably, large K_{10} values i.e. sands, loamy sands, sandy loams, loams and silt loams). Even for this dataset, dispersivity was slightly (but not significantly) dependent on scale and transport distance. Omitting experiments carried out on small cores and for travel distances less than 50 cm, gave a median dispersivity of 3.4 cm, with no correlation to textural class. This value is used.

3 CONCLUSIONS AND PERSPECTIVES

This report has described a logically consistent and complete set of parameterisation algorithms for the dual-permeability model MACRO that allow simulations of water flow and solute transport in soil profiles, using only widely available soil survey data as input. The use of such pedotransfer routines introduces uncertainties into the predictions, which should be quantified, for example by comparing model predictions with measured transport in undisturbed soil columns or lysimeters containing a wide range of different soil types. Work in this direction is in progress within the FOOTPRINT project.

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