

DRAINAGE MODELS AND MACROPOROUS SOILS – REPORT OF A SETAC WORKSHOP

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Introduction

In the procedure for the registration of plant protection products at the EU level and at the member state level, simulation models are used to assess the fate of these products in the soil. Such models should contain a state-of-the-art description of relevant processes and factors affecting pesticide losses to surface water and groundwater. Preferential flow is an important process which can significantly affect the leaching of plant protection products through soil (Flury, 1996; Jarvis, 2007), especially the fine-textured macroporous soils that are usually artificially drained for agriculture. Preferential flow is considered in the FOCUS Surface Water Scenarios (FOCUS, 2001), where the macropore flow model MACRO is currently used to predict the fate of plant protection products in soil and the discharge of water and these substances and relevant metabolites to surface water via drains. In contrast, preferential flow is currently only taken into account in one of the scenarios used for leaching to groundwater (again, using the MACRO model). However, the EFSA opinion on the Revised Groundwater scenarios for the EU states that this process may have a significant effect on leaching to groundwater in soils with macropores (EFSA, 2013).

As science develops, models should be reviewed from time to time and new developments considered for inclusion in these models. In this way the models that are being used in the registration process remain state-of-the-art and meet the requirements for a high quality assessment of the environmental impact of plant protection products. The FOCUS surface water scenarios and models were developed and parameterized in the period 1997-2001. A review of how the relevant processes are treated in the model currently used in the registration procedure for drainage inputs (i.e. MACRO) would therefore be timely. It is also evident that other models that can describe the fate and behaviour of plant protection products in drained macroporous soils (e.g. HYDRUS, PEARL) should also be reviewed.

A scientific SETAC Workshop was organised in Vienna, Austria, from 23 to 24 October 2014 on drainage models and macroporous soils. This workshop was hosted by the Austrian Agency for Health and Food Safety (AGES) at their facilities in Vienna. The meeting was jointly organised by Erik van den Berg (Alterra, The Netherlands), Bernd Gottesbüren (BASF SE, Germany), Nick Jarvis (SLU, Sweden), Anton Poot (Ctgb, The Netherlands) and Klaus Hammel (Bayer Crop Science, Germany). The Workshop Organizing Committee invited 25-30 scientists that are actively involved in research on the fate of plant protection products in macroporous soils. Scientists from different disciplines were invited: environmental chemistry, hydrology, soil physics, agronomy etc. In addition, representatives from industry, registration authorities and consultancies were also invited to attend to broaden the expertise in the area of the use of drainage models for registration purposes.

The workshop program addressed the following four topics:

- Assessment of the validation status of models that are available at present for the description of the fate of plant protection products in macroporous soils and the discharge from these soils into surface water via drains
- Assess the possibilities for improvement of models for drainage in macroporous soils based on the outcome of model tests that have been done to date
- Make recommendations for improvement of model concepts for the description of macropore flow in soils
- Make recommendations for the data requirements needed to test the improved model concepts

The workshop programme consisted of a combination of formal presentations and informal discussions. Two key-note presentations (by Jirka Šimůnek from the University of California Riverside, U.S.A and Jan Vanderborght from the Forschungszentrum Jülich, Germany) were held at the start of the workshop as a starting point for the discussion. These two talks form the basis for the state-of-the-art presentation given in the following section. During the plenary sessions, several participants were given the opportunity to give a short presentation on the topics to be addressed in the session. The programme of the workshop is given in Appendix 1, along with a list of invited participants in Appendix 2.

Current state-of-the-art of models to assess drainage losses of pesticides to surface water in macroporous soils

Several reviews have been published recently on modelling preferential flow and solute transport (e.g. Šimůnek et al., 2003; Gerke, 2006; Šimůnek and Van Genuchten, 2008; Köhne et al., 2009a,b). A brief summary follows of the main approaches that have been adopted in models that are suitable for our purpose, in that they can be used to simulate long-term transient water flow and pesticide transport under field conditions.

Preferential flow

Preferential flow in soils can be modelled in different ways. The simplest approach for preferential flow in macroporous soils is based on a one-dimensional soil system (see Fig 1). Two-domain models can be described either with dual porosity concepts (Šimůnek and Van Genuchten, 2008), where one of the domains is 'immobile', functioning only as a store of either water and/or solute, or with dual-permeability concepts (e.g. Jarvis et al., 1991; Gerke and van Genuchten, 1993a,b), where water and solute are mobile in both domains (e.g. MACRO, Larsbo et al., 2005; HYDRUS, Šimůnek et al., 2008). One of these domains has a high flow capacity and low storage capacity to represent macropores or fissures, while the other has a low flow capacity and high storage capacity (micropores or matrix). The HYDRUS-1D model allows all these options to describe preferential flow/transport (Fig. 2): a dual-permeability approach where non-equilibrium conditions are assumed for both water flow and solute transport in fast and slow water flow domains (Gerke and van Genuchten, 1993a,b) and two kinds of dual-porosity approaches: 1) uniform water flow simulated with Richards equation linked to non-equilibrium conditions for solute transport (a so-called mobile-immobile model) or 2) a dual-porosity approach which accounts for exchange of both water and solute between mobile and immobile regions. Sorption can be described assuming equilibrium conditions or non-equilibrium conditions with a one-site kinetic model, a two-site model (i.e.

one equilibrium sorption domain and one kinetic sorption domain), or a model with two kinetic sites (Šimůnek and van Genuchten, 2008) (Fig. 3). The MACRO model (Larsbo et al., 2005) currently used in EU registration is a 1D dual-permeability model similar in many ways to HYDRUS-1D. However, in MACRO flow in the macropore region is calculated with a kinematic wave equation (Germann, 1985; Beven and Germann, 2013) assuming gravity-driven flow, rather than Richards' equation. This parsimonious approach only requires three additional parameters to simulate water flow in macropores (the macroporosity, saturated macropore hydraulic conductivity and the kinematic exponent, which is supposed to reflect macropore size distribution, connectivity and tortuosity). The general validation status of MACRO has been discussed and summarized by Köhne et al. (2009a,b).

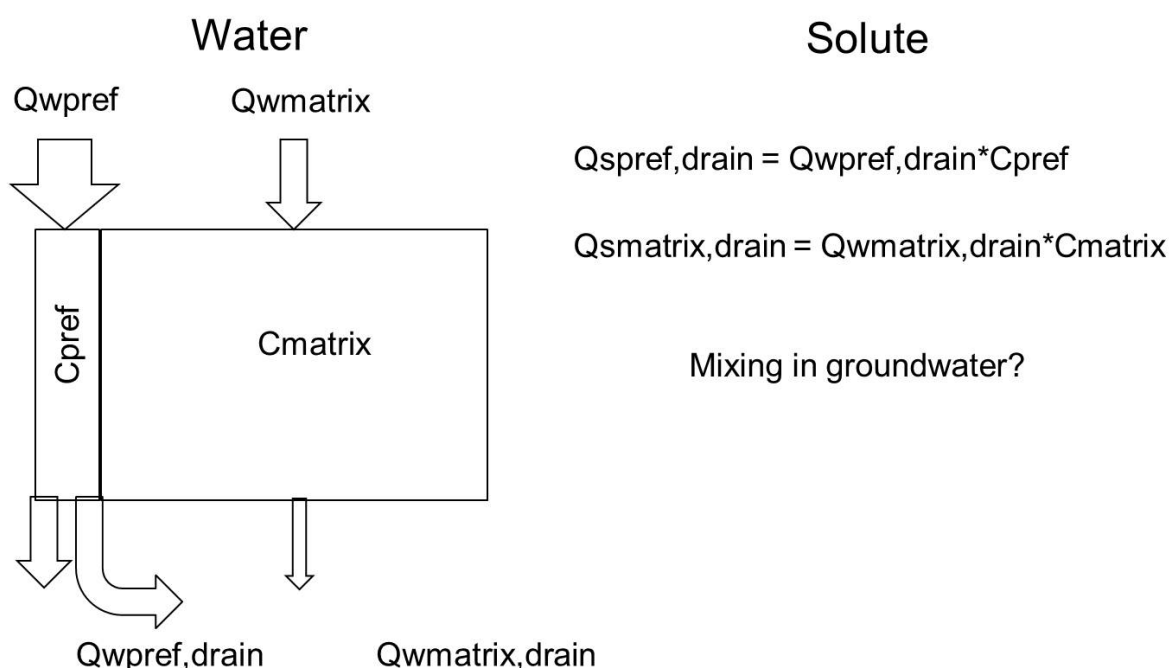


Figure 1 Description of water and solute transfer to drains as applied in 1D models.

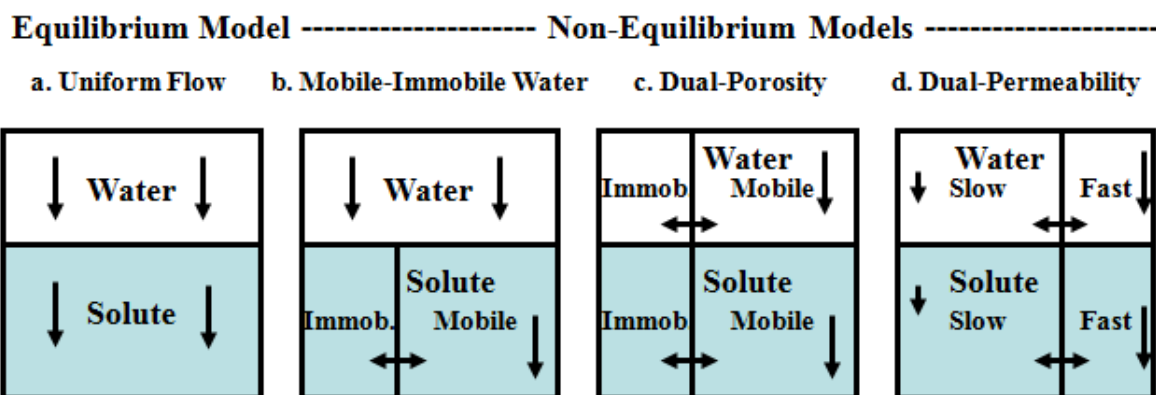


Figure 2. Conceptual physical non-equilibrium models for water flow and solute transport in HYDRUS.

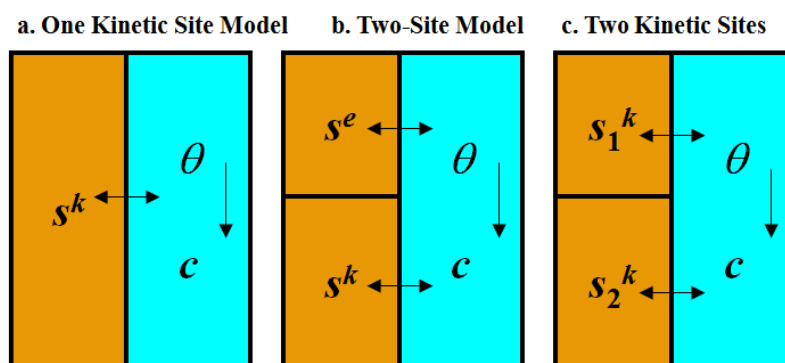


Figure 3. Conceptual chemical non-equilibrium models for reactive solute transport in HYDRUS.

Although two-domain models can easily be set up to describe soil layers or horizons where there is no functioning macroporosity (e.g. structureless single-grain soil, a plough pan or massive soil layers below root depth), they do assume that any macropores present are perfectly connected in the vertical direction. Preferential flow in the coupled PEARL-SWAP models (Tiktak et al., 2012) is essentially based on a three-domain concept, as it distinguishes two macropore domains: a by-pass domain which is connected to the base of the macroporous part of the profile and an internal catchment domain that reflects the presence of dead-end pores as shown in Figure 4. The potential importance of the internal catchment was demonstrated by Rosenbom et al. (2009) who applied the dye tracers acid yellow 7 and sulforhodamine B to macroporous soil. They found that water and solutes infiltrated less deep in autumn when the water table was higher, because some dead-end macropores were already water-filled.

Soil structure is dynamic so that, in principle, the parameters of preferential flow models describing the soil macroporosity should vary with time. One process that causes changes in soil structure and hydrologic response over time is swelling and shrinking due to wetting and drying, which is especially important in clay-rich soils (Reid and Parkinson, 1984; Leeds-Harrison et al., 1986; Messing and Jarvis, 1990). Shrinking and swelling clay soils can be simulated by including a time-variable crack porosity, which depends on soil water content and the shrinkage characteristic, in addition to permanent macropores (see Leeds-Harrison et al., 1986 and descriptions in Jarvis, 1994 for the MACRO model and Hendriks et al., 1999 for the SWAP model). Other important causes of temporal changes in soil macroporosity are the impacts of tillage and traffic in cultivated topsoil, including processes such as consolidation of the loose seedbed created at sowing and surface sealing (e.g. Messing and Jarvis, 1993; Leij et al., 2002; Assouline, 2004; Schwen et al., 2011) as well as the seasonal patterns of activity of soil fauna (e.g. Daniel et al., 1997). None of these processes are currently included in preferential flow models.

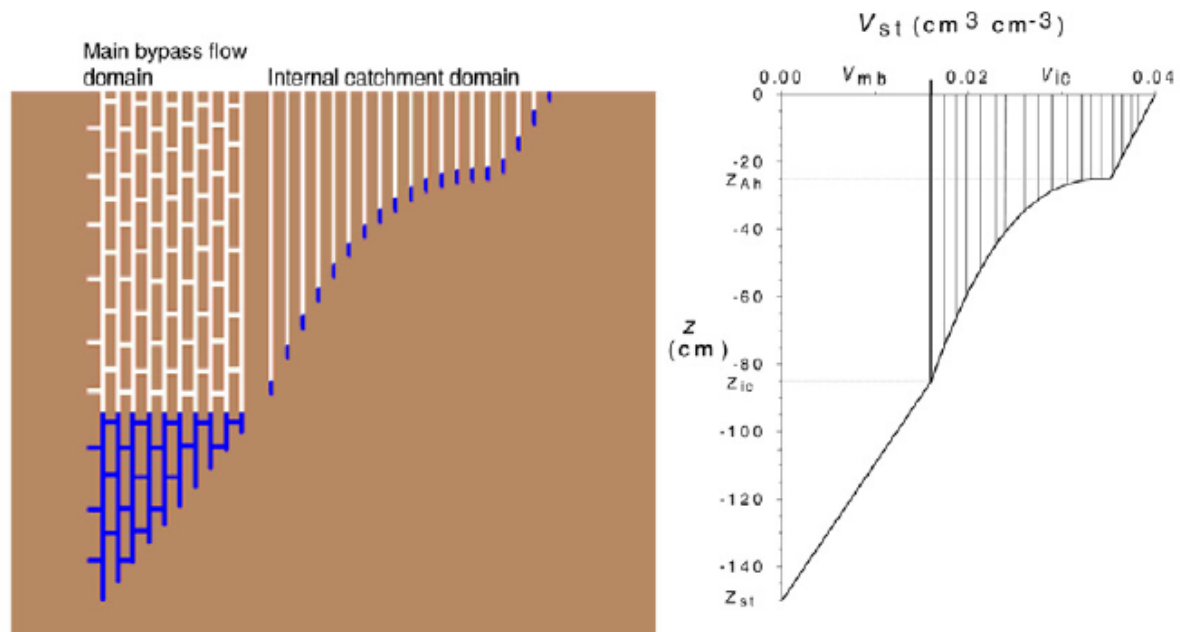


Figure 4: Presentation of the macropore domains in SWAP and PEARL.

Explicit description of macropores is possible in 2D or 3-D models (e.g. Vogel et al., 2006; Rosenbom et al., 2009), rather than the implicit representation of them in the 1D models discussed above. However, such an approach is a numerical and parameterisation challenge, not least the parameterisation of the properties of macropore surfaces, which can differ significantly from the bulk soil, with respect to flow and transport properties and chemical reactivity (e.g. Stehouwer et al. 1994; Gerke and Köhne 2002; Köhne et al., 2002). Model simulations have demonstrated, for example, that pronounced preferential flow can only be obtained when water exchange between macropore and matrix domains is reduced by assigning smaller hydraulic conductance to macropore surfaces than for the bulk soil (Gerke and van Genuchten, 1993b; Soll and Birdsell, 1998; Schlüter et al., 2012a,b).

Drainage models

When simulating flow and transport to drains, besides the vertical flow and transport pathways in the (unsaturated) soil above the groundwater table, also the horizontal flow and transport paths in the groundwater towards the drainage pipes must be considered or accounted for. It should be noted that these transport distances in the groundwater will vary from almost zero to half the distance between parallel drainage pipes. This may result in a large variation in travel times in the groundwater towards the drainage pipes. The water that enters the drains is a mixture of waters that followed different travel paths through the groundwater and that reached the groundwater table at a range of different times. The water travel time distribution is a characteristic of the soil-groundwater-drainage pipe system that can be used to describe the transport of dissolved substances. Jury and Roth (1990) used this concept to describe solute transport in soils, while Utermann et al. (1990) and Gaur et al. (2006) used it to describe transport in the coupled soil-groundwater system. The travel time distribution is equivalent to the solute concentrations that are measured in the outlet of the system (e.g. bottom of a soil profile, drain pipe) as a function of

time (i.e. the solute breakthrough curve) when solutes are applied at the soil surface as an instantaneous pulse. For the soil-groundwater system, the travel time from the soil surface to the drain pipe is split into two parts: the travel time through the soil, $pdf_{soil}(t)$ and the travel time from the groundwater table to the drain pipes, $pdf_{GW}(t)$ as illustrated in Figure 5.

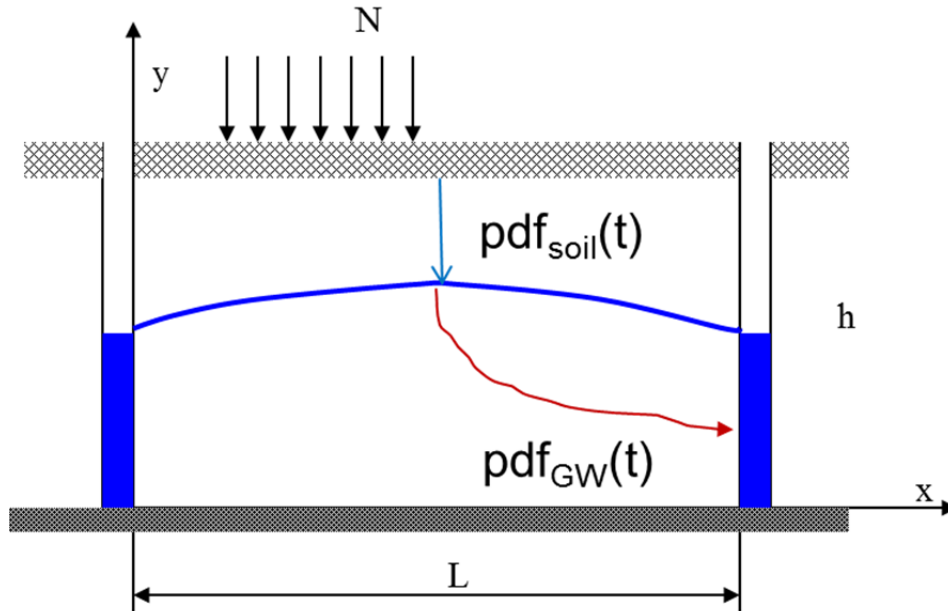


Figure 5: Sketch of the travel paths in the soil, groundwater, drain system and the travel time distributions in the soil and the groundwater.

If the travel times in the soil are not correlated with the travel times through the groundwater, the travel time distribution to the drain pipe is directly obtained from a convolution of the travel time distributions in the soil and the groundwater:

$$pdf_{Drain}(t) = \int_0^t pdf_{soil}(\tau) pdf_{GW}(t - \tau) d\tau \quad [1]$$

If the saturated zone is homogeneous, Raats (1981) showed that $pdf_{GW}(t)$ can be described as the probability density function for a completely mixed system, which corresponds to an exponential distribution:

$$pdf_{GW}(\tau) = \frac{1}{\bar{\tau}} \exp\left(-\frac{\tau}{\bar{\tau}}\right) \quad [2]$$

where $\bar{\tau}$ is given by:

$$\bar{\tau} = \frac{N}{\theta D} \quad [3]$$

Where $\bar{\tau}$ is the mean transit time, N is the recharge rate (which equals the drain discharge for steady flow) ($L T^{-1}$), θ is the porosity in the saturated zone and D (L) the thickness of the saturated zone above an impermeable base.

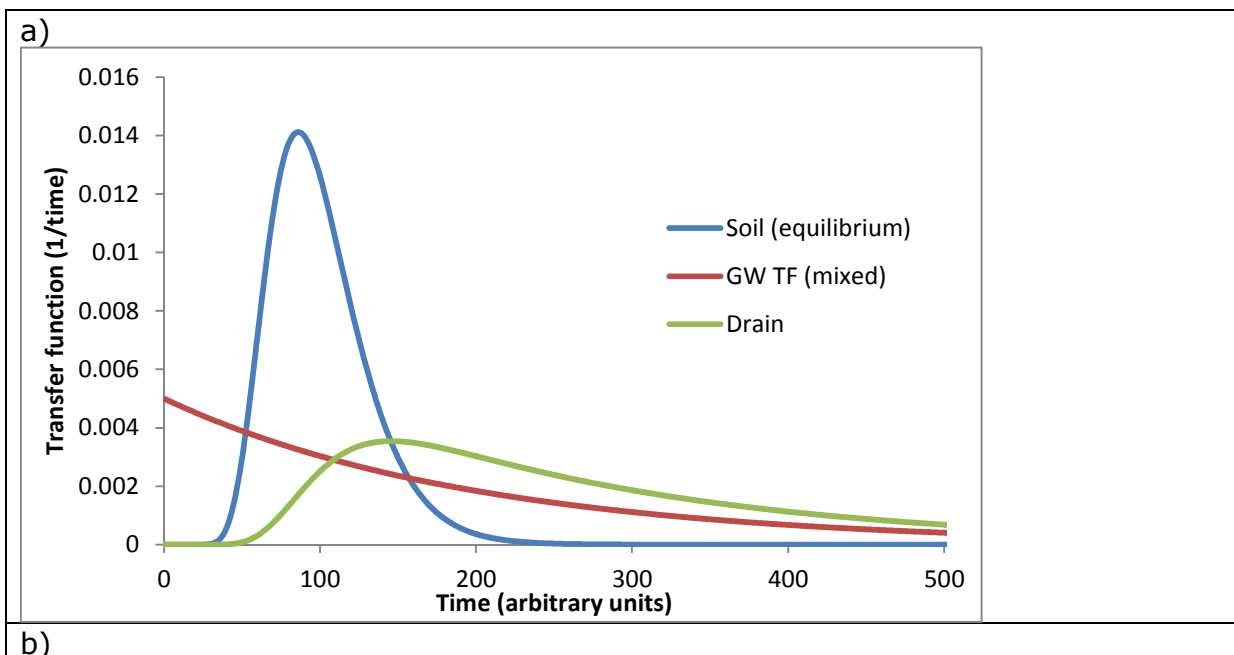
This concept can be used to illustrate the effect of different processes in a coupled unsaturated-saturated system. In Figure 6, three examples are given that represent different cases. The first example assumes no preferential flow and transport. In the second example, preferential flow/transport in the unsaturated zone is represented by a bimodal travel time distribution. In this example, no preferential flow is assumed in the groundwater (e.g. a sandy subsoil or phreatic aquifer below a loamy soil with macropores). In the third example, there is also preferential flow in the saturated zone, the preferential flow domains in the unsaturated and saturated soil are assumed to be perfectly connected and it is assumed that there is no mixing between the preferential flow domain and the matrix flow in the saturated zone. In this example, the transfer function in the groundwater consists of two parts: one for the preferential flow domain and one for the matrix flow domain. Both transfer functions are described by an exponential distribution with mean travel times given by:

$$\bar{\tau}_{GW,Pref} = \frac{N_{pref}}{\theta_{pref}D} = \frac{v_{pref}}{D} \quad [4a]$$

$$\bar{\tau}_{GW,Matrix} = \frac{N_{Matrix}}{\theta_{Matrix}D} = \frac{v_{Matrix}}{D} \quad [4b]$$

where N_{pref} and N_{matrix} are the discharges in the preferential flow and matrix domains, θ_{pref} and θ_{matrix} are the porosities in both domains and v_{pref} and v_{matrix} are the pore water velocities.

$$pdf_{Drain}(t) = \frac{N_{pref}}{N_{pref}+N_{Matrix}} \int_0^t pdf_{soil,pref}(\tau) pdf_{GW,pref}(t-\tau) d\tau + \frac{N_{matrix}}{N_{pref}+N_{Matrix}} \int_0^t pdf_{soil,matrix}(\tau) pdf_{GW,matrix}(t-\tau) d\tau \quad [5]$$



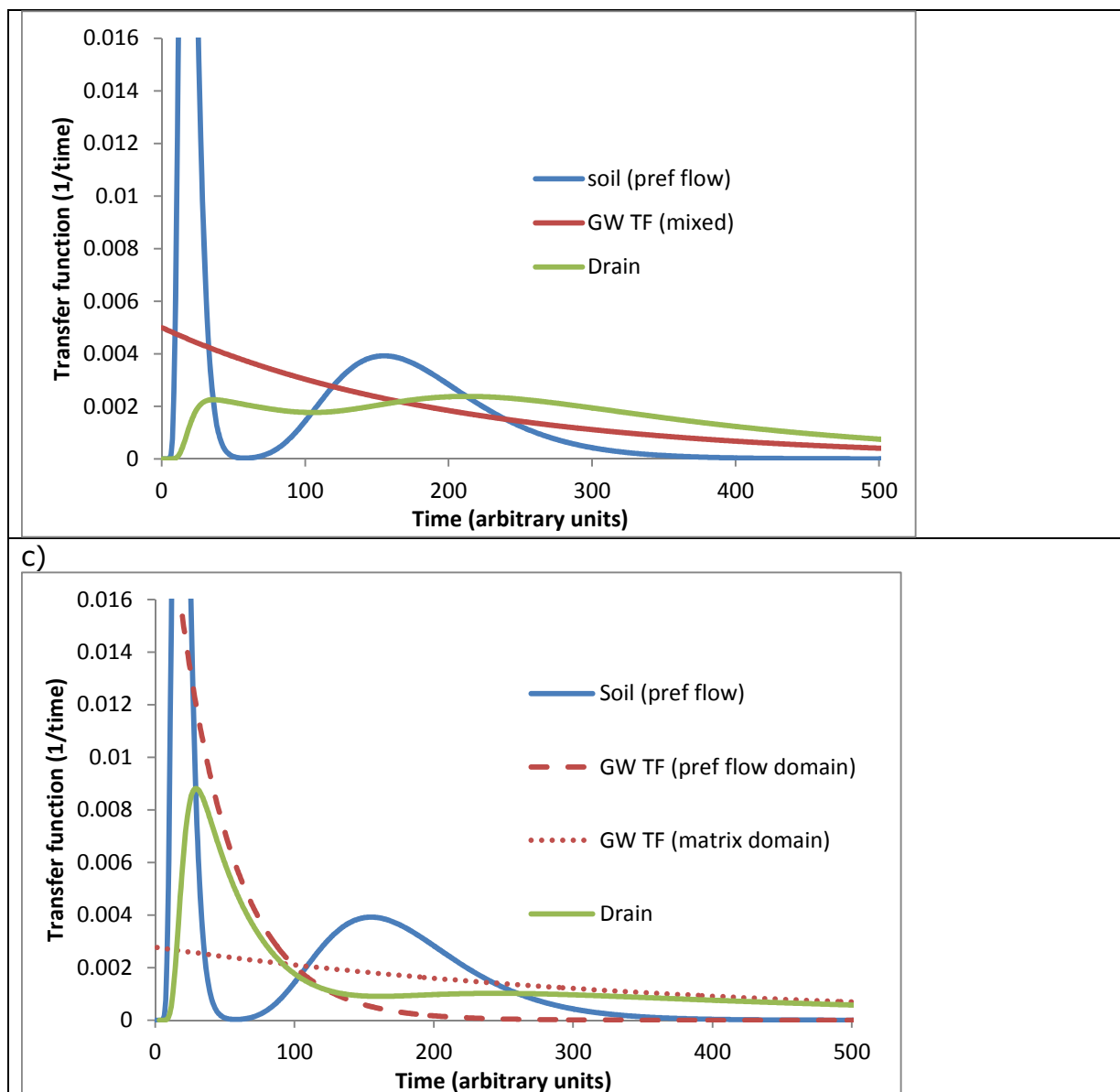


Figure 6: Three examples of travel time distributions in a coupled unsaturated-saturated system: a) equilibrium transport in unsaturated soil and groundwater, b) preferential flow in unsaturated soil and equilibrium transport in the groundwater, c) preferential flow in both unsaturated soil and groundwater.

These simple examples demonstrate in a qualitative way that:

- (i) Concentration distributions are smoothed out in the drain pipe compared with the bottom of the soil profile. This smoothing is the result of the different travel times in the groundwater.
- (ii) Preferential transport in the saturated zone leads to considerably larger peak concentrations.
- (iii) When preferential flow occurs only in the unsaturated zone, the first peak is diluted considerably by mixing in the groundwater but the peak arrival time is not affected.

These examples indicate that the way flow and transport processes in the saturated zone are represented in a model has important consequences for the prediction of concentrations in drain pipes. It should be remembered that one underlying assumption in this analysis is that the soil is homogeneous and

isotropic. This may be a reasonable description for some situations, for example in the case of homogeneous alluvial sediments located in low-lying discharge areas in the landscape. However, macroporous clay soils, which represent the worst-case scenario for pesticide losses to drains, are usually layered and therefore highly heterogeneous with respect to permeability in the vertical direction, with saturated hydraulic conductivity often decreasing by one to two orders of magnitude down the soil profile (e.g. Youngs, 1976; Messing and Jarvis, 1990; Hara et al., 1994; Alakukku et al., 2010). Indeed, the reason that these clay soils must be drained for agriculture is that the permanently saturated deeper subsoil is virtually impermeable due to the lack of structure-forming processes (i.e. swell/shrink, freeze/thaw, biotic activity). Vertical heterogeneity in hydraulic conductivity significantly alters subsurface flow pathways compared to the case of homogeneous soil. Field experiments in clay soils with slowly permeable subsoil have shown that positive pressure potentials can quickly develop in the topsoil during rainfall even when the subsoil matrix is unsaturated (i.e. perched water tables and non-equilibrium conditions develop, with saturated macropores embedded in an unsaturated matrix) and that drain discharge is dominated by shallow lateral flow in the topsoil towards permeable backfill zones above the drain (Trafford and Rycroft, 1973; Leeds-Harrison et al., 1982; Hara et al., 1994; Heppell et al., 2000; Stamm et al., 2002).

The above considerations suggest that although analytical models such as the transit time distribution approach described above can give some useful insights into the processes governing leaching in drained soils, numerical models of the system are required to describe the hydrological behaviour of heterogeneous drained macroporous soils in the field. These numerical models can be classified in terms of their dimensionality (i.e. one-, two- or three-dimensional models). Widely-used 1D numerical models include MACRO (Larsbo et al., 2005), SWAP (Van Dam et al., 2008) and HYDRUS-1D (Šimůnek et al. 2008). In such models, drainage is calculated as a sink term to the vertical 1D flow using analytical drainage equations, such as those of Hooghoudt (Hooghoudt, 1940), Ernst (Ernst 1962), or Cook (Cook et al., 2001). For homogeneous soils (i.e. without layering), vertically uniform sink terms predicted by the Hooghoudt equation are used in PEARL and HYDRUS-1D, which as noted above leads to exponential travel time distributions in the groundwater (see Eq. 2). For heterogeneous soils, the sink term in HYDRUS-1D is proportional to conductivities of individual saturated soil layers. Alternatively, HYDRUS-1D also allows to apply the total drainage flux at the bottom of the soil profile, rather than distributing it vertically along the saturated zone. When the dual-permeability approach is used, HYDRUS-1D uses the same approach as described above for each (matrix and fracture) domain. Although this approach can potentially lead to two independent water tables in each domain, the two water tables should quickly equilibrate because of the faster exchange between the two domains in the saturated zone. When preferential flow is considered in the groundwater and sink terms are derived using Hooghoudt equations with different conductivities for the preferential flow and matrix domains, two exponential travel time distributions are obtained when there is no diffusive exchange between the two domains in the groundwater. It must be noted that diffusive exchange and mixing along the trajectories in the groundwater is actually represented in 1D models when the solute plume travels downward below the groundwater table in the 1D soil profile.

In MACRO, seepage potential theory (Youngs, 1980; Leeds-Harrison et al., 1986) is applied to describe drainage from layers above drain depth. The advantage of seepage potential theory is that it explicitly accounts for the effects of vertical variations in hydraulic conductivity within the saturated zone. The approach assumes highly permeable backfill material above the drain or a fully penetrating open ditch. The second term of the Hooghoudt equation (the contribution to discharge from below drain depth) is used to calculate drainage from layers below drain depth. MACRO also allows users the option to simulate the effects of two drainage systems: parallel within-field drains, as well as open ditches surrounding the field. In keeping with the non-equilibrium nature of flow in macroporous soils, MACRO simulates drain discharge response as a function of multiple independent 'zones of saturation' that may co-exist at different depths in the soil profile (i.e. perched water) and in both matrix and macropores (see Figure. 7).

Several field tests of MACRO in drained soils have been reported (Köhne et al., 2009a,b), which demonstrate the ability of the model to match observed drain discharges as well as tracer and pesticide concentrations in drainage, including applications at several of the FOCUS drainage scenario sites (e.g. Larsson et al., 1999 and Steffens et al., 2013 for D1 (Lanna), Armstrong et al., 2000 for D2 (Brimstone), Jarvis et al., 2000 for D3 (Vredepeel) and Surdyk et al., 2007 for D5 (La Jaillière)).

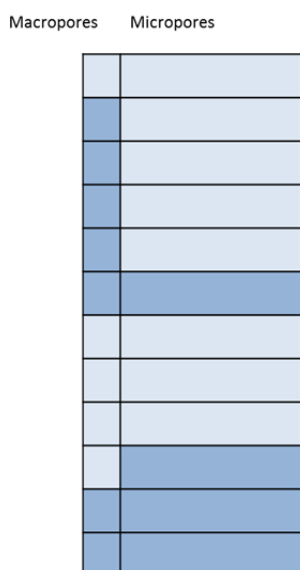


Fig. 7. Multiple saturated zones in a soil profile. Dark blue cells indicate saturation. In this example, discharge to drains is simulated by MACRO from the saturated macropores in layers 2-6 and 11-12 and from the micropores in layers 6, 11 and 12 (but not layer 10 because the pressure potential at micropore saturation is not zero).

The SWAP model comprises two different methods for calculating drain discharge:

1. use drainage formula of Hooghoudt or Ernst for a single drainage system (open or tile drain): five field drainage situations are considered in SWAP;
2. use drainage and infiltration (sub-irrigation) resistance for a single or a multiple drainage system (Fig. 8). Up to five drainage levels can be used simultaneously. Drainage systems may consist of open drains, tile drains or

an interflow system (rapid lateral drainage through the first decimetre(s) of the soil profile) at the top of the profile. The slopes of the lines represent the cumulative drainage resistances starting from the deepest drainage system of order 1 (after Massop and de Wit, 1994).

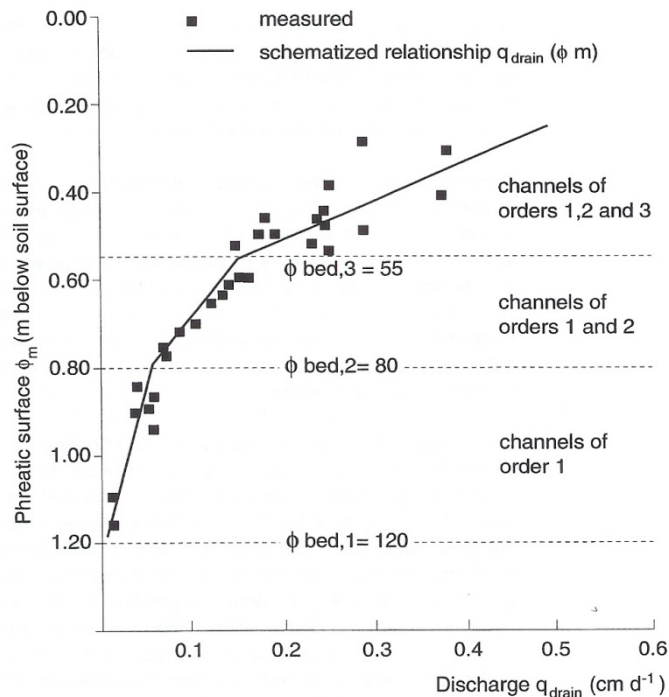


Figure 8 Example of a drain discharge relation with three drainage levels (channels). Shown is q_{drain} as function of mean phreatic surface Φ_m . The drainage basis of each channel is denoted as 'bed' in cm below soil surface.

SWAP uses a pseudo-2D approach for distributing drainage fluxes with depth. This distribution is used to describe the travel time distribution of drainage water in an implicit manner. The approach is based on the transmissivity KD (the product of saturated conductivity K and thickness D) of each discharge layer and on the magnitude of the drain flux and drain distance of each drainage system.

Drainage from the macropore system is strictly from the main bypass domain. It is described in a similar manner with a drainage resistance as method 2 of calculating drain discharge from the soil matrix but (at present) only for one drainage system. In case of widening and narrowing cracks due to swelling and shrinking of the soil matrix, the input drainage resistance represents a reference resistance that may decrease when cracks are widening and increase when cracks are narrowing. This adjustment of the resistance is based on a slit model for conductivity. Drain flux distribution with depth and travelling time distribution are described in the same way as for the soil matrix.

More complex and advanced models consider two-dimensional flow, HYDRUS (2D/3D) (Šimůnek et al., 2008), VS2D (Healy, 2008) and Tough2 (Pruess, 1991). For homogeneous soils in the lateral dimensions, the parameterization of 2D models is similar to that of 1D-models. However, due to required fine numerical discretizations (both spatial and temporal), computational times may be very large, while numerical stability may be a problem. Perhaps for these

reasons, their applications to modeling transport of pesticides to tile drains have been rather limited. Using the Chain-2D model (a predecessor to Hydrus (2D/3D)), Mohanty et al. (1998) investigated preferential flow of water and nitrate to tile drains in flood-irrigated systems. A piece-wise continuous function for near-saturated hydraulic conductivity gave a reasonable match with the observed water and drainage fluxes.

Abbaspour et al. (2001) used a model called M-2D (based on SWMS-2D, a predecessor to Hydrus (2D/3D)) to simulate water flow and solute transport in a macroporous soil with tile drains. The macropore domain represented surface-connected cracks and macropores, in which water flow is one-dimensional, non-capillary, and laminar, and where solute transport is purely convective. An individual macropore was assumed to consist of a sequence of macropore nodes (macro-nodes) that extend vertically from a surface micropore node (micro-node) down to a desired depth. Water exchange between a micro-node and a corresponding macro-node was calculated as a function of the pressure head difference between the two nodes. The measurements of the first 6 months of the field experiment described by Abbaspour et al. (2001) were used for calibration. The measurements of the next 12 months were used to validate the model. The calculated drain flow and the concentration of bromide in the drain water corresponded best to the parameterization that included a macropore domain and a Hooghoudt boundary condition.

Köhne and Gerke (2005) compared the ability of two different 2D modeling approaches in HYDRUS-2D to simulate bromide transport to tile drains, an equilibrium model without preferential flow (Richards and CDE) and a dual-porosity mobile-immobile water model. The timing of the arrival of the maximum concentration of bromide in drainage calculated with the dual-porosity model corresponded well to that observed in the field. Gärdenäs et al. (2006) used HYDRUS-2D to model water flow and transport of the herbicide MCPA to tile drains in an arable soil on a hill slope. A dual-permeability approach gave the best description of the time-course of concentrations of MCPA in the drainage water. Boivin et al. (2006) compared pesticide behaviour in three soils with different textures, ranging from sandy loam to silty clay. The temporal pattern and peak concentrations of bentazone in the drainage could be reasonably well described using HYDRUS-2D with the model approach assuming mobile-immobile water.

Other applications of HYDRUS-2D to water flow in tile-drained soils were carried out by Akay et al. (2008) and Filipovic et al. (2014). Akay et al. (2008) made detailed measurements of pressure heads and discharge from an artificial drain in a soil column in the laboratory. Filipovic et al. (2014) investigated water flow in soils with different drain system designs, including tile and mole drains.

Köhne et al. (2006) compared 1D and 2D models to describe solute transport to drains in a macroporous soil. Overall the 2D model gave better results than the 1D approach. The 1D approach generally leads to larger simulated concentrations just after the application of the substance. This could be explained by the fact that the groundwater table depth that is considered in 1D models corresponds with the groundwater table depth mid-way between two drains. The solute that arrives the earliest at the drain pipe is that which is applied just above the drain

pipes. In a 2D model the profile above the drain is unsaturated with larger travel distance towards the groundwater table than in the 1D model.

Boundary Conditions

The way that solute is applied has an important impact on leaching risks in macroporous soil (e.g. Kluitenberg and Horton, 1990; Kätterer et al., 2001). It is therefore important that attention is given to ensuring that the upper boundary condition in preferential flow models is treated in a physically realistic way. Gerke et al. (2007) studied the effect of the upper boundary condition on the transport of bromide to tile-drains. They showed that there was a substantial difference in the calculated peak concentration when the solute was applied to both domains or only to the matrix domain. In practice, if a pesticide is applied as a spray then it can be treated in the model as an irrigation of known intensity and duration. The modeller does not need to specify 'a priori' which domain the pesticide enters, since this will depend on the antecedent soil moisture condition. If the soil is not close to saturation (which it is not likely to be), all the pesticide should enter the soil matrix.

A crucial aspect of the upper boundary condition in macroporous soils is the transfer of pesticides into surface water that does not infiltrate into the soil matrix but instead infiltrates into the preferential flow domain (Jarvis, 2007). When a heavy rain event occurs after the substance has been applied, water that runs off from the matrix and infiltrates into the preferential flow domain would have a zero concentration if there is no transfer of the substance from resident water stored in the upper layers of the soil matrix domain. How much of the substance that enters into the preferential flow domain is sensitive to how this transfer is described in the models. HYDRUS does not account for solute exchange between resident soil water and incoming precipitation so that the flux concentration that enters both domains is equal to the concentration of the substance in the rain or irrigation water. Both MACRO and PEARL assume that the incoming rain mixes with the resident soil water within a certain mixing depth, before any excess water is routed into the macropore domain, a concept that was borrowed from surface runoff models (Jarvis, 1994). Kätterer et al. (2001) showed that the mixing depth concept implemented in MACRO could, in all but one case, accurately simulate solute leaching in column experiments carried out with two contrasting initial conditions (dry and wet soil) with multiple solutes, including those which were indigenous to the soil as well as tracers applied in irrigation or soil-incorporated.

It is also worth noting here that the numerical discretization of the soil profile close to the surface also influences how much of the applied pesticide can be routed into macropores from the mixing depth soon after application. A coarse discretization artificially disperses and dilutes the pesticide in the surface layers immediately following application. This has little consequence for predictions of leaching in the absence of preferential flow, but recent experience with the MACRO model shows that it can be critical in two-region models based on the mixing depth concept. Early sensitivity analyses with MACRO showed that the mixing depth was not one of the more sensitive parameters for leaching in macroporous soils (Dubus and Brown, 2002). However, this conclusion may have been affected by a rather coarse numerical discretization, which was required by the explicit finite difference scheme in MACRO at that time.

The bottom boundary condition has a strong influence on the soil water balance and the partitioning between recharge and drainage in macroporous soils. The bottom boundary conditions available in current 1D models are quite similar. In MACRO, there are five bottom boundary conditions (i.e. zero flux, constant hydraulic gradient, water table in the profile, fixed pressure head or a lysimeter boundary condition). SWAP comprises eight bottom boundary conditions: zero flux, prescribed groundwater level, prescribed pressure head, prescribed flux, flux calculated from piezometric level in the aquifer, flux as a function of groundwater level, free drainage and free outflow at the soil-air interface. In HYDRUS, there are a number of bottom boundary conditions, including constant and time-variable pressure heads or water fluxes, free drainage, deep drainage, horizontal drains, and/or a seepage face (which can be applied at the bottom of lysimeters), but only the "Horizontal Drains" boundary condition applies to drained soils. The most relevant bottom boundary conditions for drained soils in the field are fixed or time-variable pressure heads or a flow boundary condition that maintains a fluctuating water table in the simulated profile (e.g. with outflows calculated as a function of the water table height).

Recent developments in the domain of modelling drainage losses of pesticides to surface water in macroporous soils

Horst Gerke (ZALF, Germany) started his presentation entitled **"Characterization of intact biopore walls and aggregate coatings for describing local non-equilibrium and inter-domain mass transfer"** with a report on a field experiment in which the transport of bromide was measured from the site of application towards the drain. This drain experiment was parameterised using a 2D dual permeability flow model. The results showed that local redistribution of water and solutes at the soil surface (and at subsurface layer boundaries) needs more attention. For a description of mass transfer between the macropore domain and the soil matrix domain the surface of the biopore walls and aggregate surfaces have to be characterised. A method was presented to characterise the surface characteristics using diffuse reflectance spectroscopy. An indicator for the composition of organic matter (OM) at biopore and aggregate surfaces was presented based on the ratio between aliphatic (hydrophobic) and carboxylic (hydrophilic) groups in OM (Ellerbrock and Gerke, 2013 and Leue et al., 2013; see Figure 9). Next maps of local organic matter composition of different surfaces were presented. Uncoated surfaces were highly wettable, other areas displayed potential water repellency.

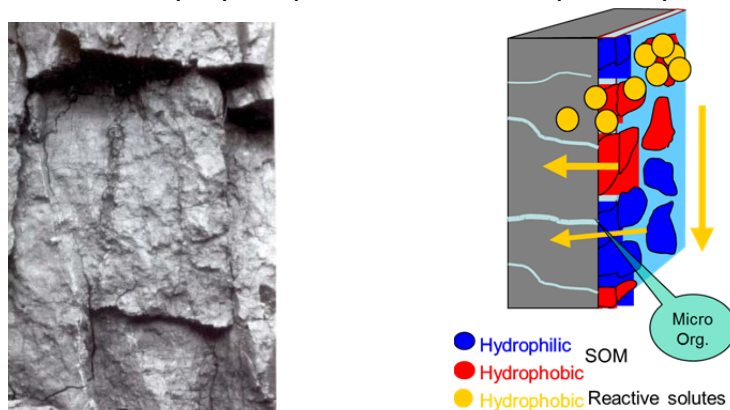


Figure 9: Clay structural elements (left) and conceptualization of OM and sorption properties at structural surfaces (right).

However, a description of reactive transport in macropore networks with locally heterogeneous properties remains challenging. Sorption along preferential flow paths is mostly restricted to the intact surfaces. As sorption properties cannot be derived from data obtained by using mixed samples, new sampling techniques are needed. Further, a characterization of the surfaces of the macropore network may make it possible to establish a link to soil management and crop production.

Further investigations need to be done how to determine the 3D-distribution of wettability in the structural pore space and how to combine pore structural geometry and quantification with properties at (macro-)pore surfaces. Other areas of interest are to assess in what way land use and soil management can modify the composition of organic matter and organo-mineral complexes at structural surfaces. Further the relation between coating properties with soil biological activity needs further attention.

In the presentation "**Biopores: earthworm influence on soil hydrology and drainage**" **Loes van Schaik** stated that macropores are strongly variable in space and time, in particular for biopores. Therefore it is of interest to study earthworm ecology. In a study on the extent of occurrence of earthworms and the effectiveness of macropores in a tillage and no-tillage system, she counted the macropores in soil after soil excavation. Based on the ecology of earthworms, she distinguished 3 classes of earthworms, epigeic (top few cm, biopores oriented horizontal), endogenic (top 20-25 cm, biopores oriented horizontal as well as vertical) and anecic (biopores oriented vertical, can be deeper than 0.5 m). In addition she applied rainfall experiments with a dye tracer. The macropores were partitioned in 3 size groups: < 2 mm, 2-6 mm and > 6 mm. Macropores were counted and classified as stained (hydrologically effective) or non-stained. Tillage (top 20 cm) had no effect on the occurrence of anecic type earthworms, but the occurrence of epigeic earthworms was greatly reduced. Furthermore, there was a significant relationship between the total number of macropores and the abundance of earthworms, e.g. the earthworms in the anecic class at all measurement depths (i.e. 10, 30 and 50 cm). Ploughing had a significant effect on the abundance of epigeic class earthworms, but no effect on the abundance of anecic class earthworms (Van Schaik et al., 2010). From the results it could be demonstrated that hydrological effectiveness decreases with depth (see Figure 10) and that the hydrological effectiveness decreases with pore size.

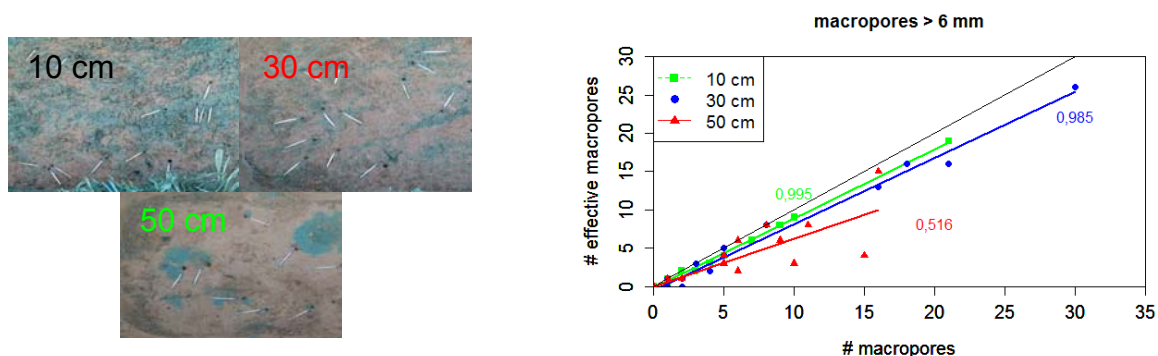


Figure 10: Correlation between the number of macropores > 6 mm diameter and the number of effective macropores.

The spatio-temporal distribution of macropores depends on rate of burrowing and disturbance, such as tillage. The geometry of macropores, i.e. the diameter, depth, length, and orientation, depend on earthworm ecological types and some habitat characteristics such as organic matter quantity. The connectivity of the local macropore networks determine the hydrological effectivity of macropores first at field scale and later on at hillslope to catchment scale.

An important aspect are the surface characteristics of the macropores. This determines the interaction between macropores and soil matrix and acts as a microbiological hotspot, where adsorption and biodegradation of solutes are concentrated.

In the presentation of **Annette Rosenbom** entitled “**Can MACRO describe drainage at arable PLAP-fields during unsaturated conditions and snow melt?**” she showed results of field experiments included in the Danish Pesticide leaching assessment programme (PLAP). The locations of these sites are presented in Figure 11. The MACRO model was parameterized for the three arable soils.



Figure 11. Location of PLAP fields in Denmark

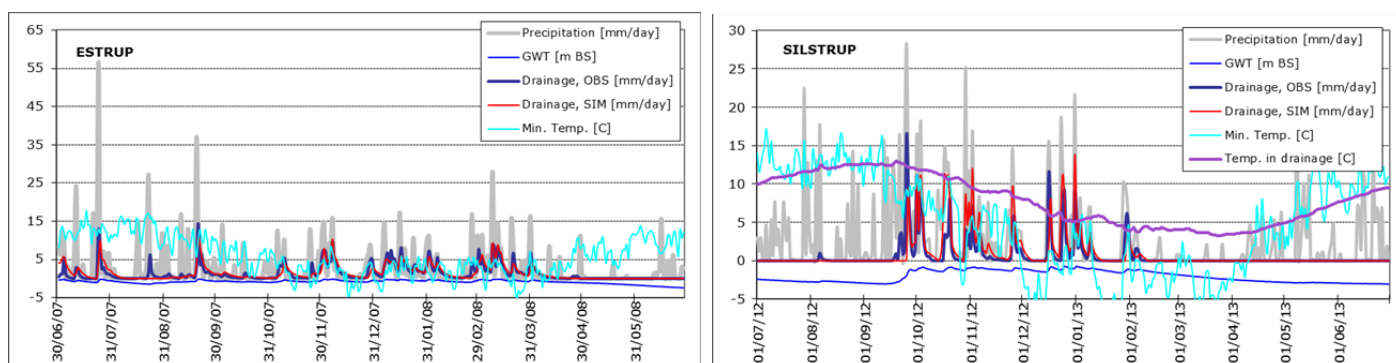


Figure 12: Simulated and measured drain flow in 2 arable soils in Denmark.

Key results on these experiments are shown in Figure 12. A comparison between measured drainfluxes in a one year period showed overall good results, but for some conditions substantial differences were observed, e.g. during snow melt. Under these conditions it is important to have information on the infiltration on the soil and the extent of surface runoff. However it remains difficult to predict events with rapid preferential flow. Therefore, further study is needed to investigate whether it is possible to delineate surface conditions leading to such events. Further challenges are how to optimize the simulation of flow in the discontinuities (wormholes + fractures) contained in unsaturated soils. As such discontinuities have different surface characteristics it is of interest to study whether the presence of a surface coating can be categorized for different discontinuities.

In a presentation entitled “**MACRO: strengths and limitations**” **N. Jarvis** (SLU, Sweden) gave his views on the further development of the MACRO model. Current ongoing developments include the incorporation of two additional processes i.) soil freeze/thaw, and ii.) temporal variations in soil hydraulic properties in tilled soils and seal development. In future model developments, it may also be relevant to address water repellency, because this can enhance macropore flow.

In the presentation entitled “**Current and intended actions for improving the SWAP model**” **R. Hendriks** (Alterra, Netherlands) elaborated the further development of the SWAP model. Four topics were mentioned: a) coupling with detailed crop model WOFOST, b) evapotranspiration partitioning during crop development, c) root water extraction under combined water and osmotic stress and d) macropore flow. In the description of evapotranspiration a physically based approach will be followed, without the use of crop factors. For stress factors water, lack of oxygen, and salinity common reduction functions will be developed.

For macropore flow, improvements would involve a rate dependent vertical flow of water (kinematic wave). Another improvement is about hysteresis during drying-wetting/swelling-shrinking. This is relevant because shrinkage cracks in heavy clays disappear during winter time, which blocks flow to drains. Other phenomena related to hysteresis in swelling imply prolonged subsidence of peat soil surfaces and peat dike crowns due to shrinkage of the peat. The approach for improvement could involve hysteresis during drying/wetting cycle and an extra time dependent swell factor.

Another important topic is the effect of biopores on macropore flow. Biopores can reduce runoff and peak flows. These biopores contribute to the water flow and solute transport in the bypass domain.

In a presentation entitled “**What are appropriate upper boundary conditions for modelling preferential flow in the Swiss Plateau?**” **C. Stamm** (EAWAG, Switzerland) raised questions how to address this issue. The first step is to describe the link between surface runoff and transport to subsurface drains. This has consequences for defining upper boundary conditions as well as for transport to drains.

A catchment on the Swiss plateau was selected for a field study. The connectivity of subareas to streams and shortcuts is shown in Fig 13.



Figure13: Connectivity of transport elements (left) and retention in drained sink and shortcuts (right).

The link between surface runoff and transport to subsurface drains comprises different pathways: surface runoff retained in internal sinks, transport through natural macropores and transport through artificial short-cuts like manholes (See Figure 13 right).

The consequences of the combination of these pathways is that homogeneous input at the upper boundary not realistic (exclusion of dominant worst-case combination). This is illustrated in Figure 14.

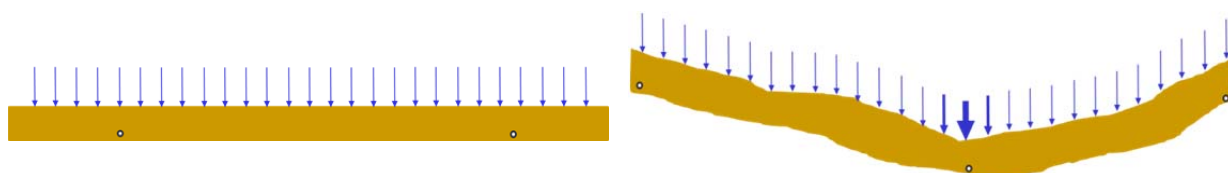


Figure 14: Schematic view of upper boundary conditions: homogeneous rainfall (left) and heterogeneous rainfall (right).

It should be noted that short-cuts are even more efficient in transporting pesticides than macropores. The following equation can be derived based on the analysis of the pathways leading to drain flow:

$$I_{\text{drain}} = I_{\text{macro}} + I_{\text{sinks}} + I_{\text{shortcut}}$$

For further development of the approach for the Swiss catchment it is of interest to collect data on studies in other landscapes. In addition to drain flow, the coupling with surface runoff modelling could be investigated. For future investigations on other catchments it is recommended to find out how landscape

metrics can be used for assessing the heterogeneity of preferential flow at the catchment scale.

In the presentation entitled **"A spatially distributed model of pesticide movement in Dutch macroporous soils"** A. Tiktak (PBL, Netherlands) described the methodology to derive a schematisation for macroporous soils in the Netherlands. About 40 % of the Netherlands is tile-drained and as the peak concentration of pesticides in surface water cannot be described with the classical CDE, a macropore version of GeoPEARL was needed. Therefore, pedotransfer functions were developed that relate geometry to basic soil properties. Four key parameters describing geometry were defined: 1) the maximum depth of all macropores, 2) the maximum depth of internal catchment domain, 3) the volume of permanent macropores at soil surface and 4) the depth of the plough layer (See Figure 15, left).

The maximum macropore depth was set equal to the mean lowest groundwater table. No ripening of clay occurs below this depth, so no structural shrinkage cracks are present. In addition, the macropore depth is generally deeper than the drain depth. The maximum depth of the internal catchment domain was set equal to the drain depth. So water captured above this depth must re-infiltrate into the soil before it can reach drainpipes.

A method was developed to estimate the volume of permanent macropores at soil surface. In Dutch clay soils, permanent macropores generally originate from structural shrinkage, so a two step approach was followed. First the shrinkage potential (coefficient of linear extensibility, COLE) was estimated from the organic matter and clay contents. Next the volume of permanent macropores at soil surface was calculated from the COLE parameter. For three sites, the correlation of the calculated COLE value with the measured value is presented in the RHS of Figure 15.

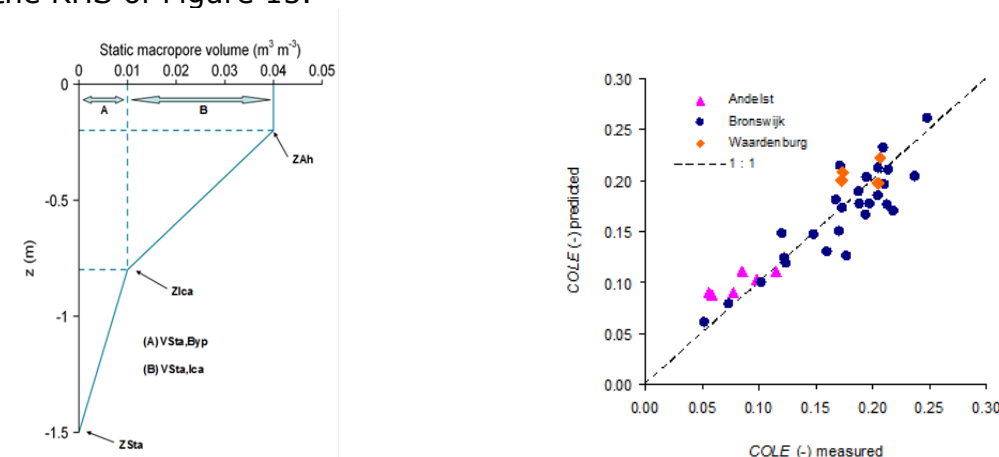


Figure 15. The macropore volume as a function of soil depth (left) and the correlation between measured and predicted COLE values (right).

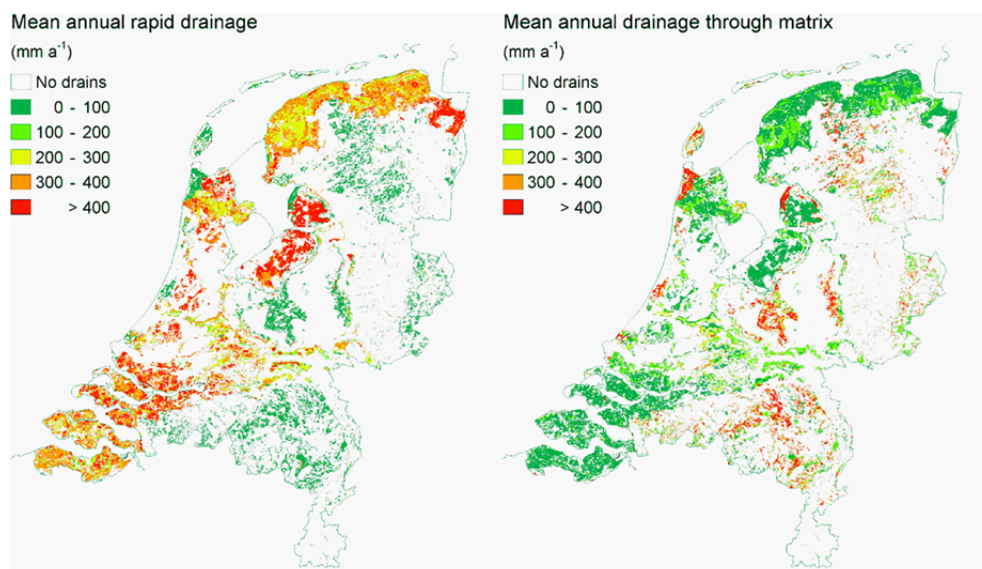


Figure 16. Drainage in agricultural soils: rapid drainage (left) and matrix drainage (right).

The results of the calculation of annual drainage (mm) using GeoPEARL are shown in Figure 16. These results show that in sandy soils matrix drainage is most important and in clay soils rapid drainage is the most important.

The approach developed for the Netherlands could be used for assessments at the EU scale. It is yet unknown whether there is sufficient soil structural information available to perform such exercises at the European level. An assessment need to be made what the most important data limitations are and how to proceed to obtain these data.

Although the calculated results seem plausible, the target output needed for pesticide authorisation has yet to be defined, while taking into account the uncertainty in the input data.

Discussion sessions of the Workshop

Session A: Process description of macropore flow and analysis of model concepts
In this session the processes to be included in models for drainage in macroporous soils were discussed. These are:

- surface routing for water and solute
- mass exchange between domains
- seasonal dynamics of macropore system
- appropriate drainage description: Hooghoudt or analytical solution
- flow dynamics in macropores
- representation of macropore system: bypass system, this can locally be different
- plants, including dynamic root system
- snow and frost
- metabolites
- option for 2D/3D; specification in which cases 2D/3D models can be used

During this discussion the following remarks were made:

- MACRO can handle ploughing and swelling/shrinking, but this module needs further testing.
- 2D models can be taken as a reference for the performance of 1D models.
- Mass exchange between the different domains is very important, but this process is difficult to parameterize.
- Dynamics of bioturbation are an important topic but this process is not yet included in the models.
- The partitioning of the amount applied to the soil between the bypass domain and the internal catchment domain is important but not yet thoroughly investigated.

Session B: Field and lab experiments for improvement of validation status

In this session the discussion was focused on experiments needed to increase the validation status of current models.

The following items were identified as important for testing:

- Definition of upper boundary in experiments: also consider lower infiltration rates.
 → smaller macropores may be environmentally relevant
 → problem of continuity and variability maybe less
 → parameters may be determined in column scale experiments.
 → Field experiments are still necessary to characterize connectivity
- Temporal variability of soil surface properties (surface sealing, splash erosion, tillage)
- How would experiments have to be designed now with all the knowledge that became available since the parameterization of the Focus scenarios?
 → old experiments are reanalyzed giving new insights of the processes but the representativity of the knowledge is not increased
 → what additional measurements would we gather from new experiments.
 → High spatial and temporal resolution data and non-invasive methods (both at column and field-scale).
- How to characterize the structure and processes below the groundwater table where lateral flow is dominant?

Session C: Model improvements

In this session the discussion was focused on future model improvements.

The following propositions were made:

- General requirement -> model output should be independent of numerical discretisation
- Mixing depth, concept may be good but the question is how to parameterize it.
- Temporal variability of surface processes:
 - snow melt in spring → drainage even though soil is still frozen;
 - infiltration capacity
- Temporal variability of other processes:
 - macropore system (biopores) in the plough layer/pan → but scalable to EU level?
- Downscaling of daily precipitation → is the concept still correct (it is appreciated that the models can do it but the question is how it is implemented)

- Run-On modeling/ponds → no real modeling concept out there; however, use a model first too see how relevant this process is (impact assessment) (do you need this surface process to explain your observations?)

Session D: experiments for model improvements

In this session the discussion was focused on experiments to test the improved models. The following suggestions were made:

- Lab experiments
 - European agricultural contextualisation of simulated conditions is critical
 - Potentially more useful than field experiments for understanding processes of mass exchange
 - Role of macropore type/soil texture/land use in determining mass exchange processes requires better understanding
 - Any lab based technique is required to be scalable both conceptually (lab→field→catchment →continent) and logistically (sample throughput/cost)
 - Study of existing legacy lab studies/samples provides opportunity for cost efficiencies and can augment new studies (specific mention of resin studies)
 - Requirement that a range of environmentally relevant upper boundary conditions are utilised (not just the extremes)
 - Lab techniques such as CT are powerful, however, throughput and conceptual scaling issues need to be addressed.
 - Lab experiment to better understand distribution of different macropores under different simulated land management regimes/soil textures/EU regions. This should also examine earthworm type/distribution.
- Field Experiments:
 - Existing field studies:
 - Cohort of well instrumented, long duration field experiments represent a critical resource
 - Require better understanding of each site's ranking within a pan-european risk CDF
 - In Silico: Use of ensemble modelling approach utilising MACRO, HYDRUS, SWAP and "blind" parameterisation with existing pedotransfer functions to simulate existing field studies will enable better understanding of model sensitivities
 - Interplay of combined run-off and drainage measured at Brimstone – can we make use of this/was it examined elsewhere?
 - New field studies:
 - Require understanding of each site's ranking within a pan-european risk CDF
 - Can we identify an "ideal" tracer? If not does a tracer "cocktail" present enhanced opportunities?
 - Tracer application timing critical (subsequent weather events/cropping)
 - non-invasive Geophysical, proximal or remote sensing techniques e.g. ERT (Oberdörster et al. (2010) or cross



borehole GPR (Haarder et al., 2012) give new possibilities to investigate and understand plot and field scale water flow and solute transport in soils.

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- Minimum study area size = x2 drain spacing interval

General discussion and recommendations

1D drainage models are conceptually incorrect, which introduces approximations and assumptions. The results of 1D and 2D simulations should therefore be compared for various drainage scenarios (both with and without preferential flow), in order to evaluate the errors introduced by the 1D assumption. This work would best be done with HYDRUS, because HYDRUS has both 1D and 2D options to simulate water flow to drains. Notwithstanding this, 1D models should be more conservative than 2D models and are probably accurate enough for regulatory purposes. 2D models that include preferential flow are also more difficult to use, they are very slow (with long computation times) and they are not always numerically stable. However, 2D models may be needed for cases with non-uniform flow, for instance in potato growing and in row-irrigation.

Models that include internal catchment and models that assume perfectly connected macropore networks should be compared. The spatial and temporal variation of macropore hydraulic conductivity in relation to macroporosity and connectivity also requires further attention. New non-invasive methods such as X-ray tomography may enable the variability in these soil properties to be mapped, while percolation concepts (Hunt et al., 2014) may provide a unifying theoretical framework to help analyse the data and support upscaling from the laboratory to the field.

Parameterisation of preferential flow models is a challenge. The method of parameterisation needed depends on the tier in the exposure assessment. This is most straightforward at the first tier, since four of the six first-tier surface water scenarios are based on real field sites. For example, the parameterization of MACRO for three of these scenarios (D1, D2, D3) is based on model calibration to field experiments. Pedotransfer approaches for preferential flow parameters are needed to parameterise the models at higher tiers and larger (e.g. European) scales (e.g. Jarvis et al., 2009, 2012; Tiktak et al., 2012). The uncertainties involved in this kind of predictive modelling will probably be significantly larger. The bottom boundary condition for unknown sites is not known, although it largely controls the partitioning between groundwater recharge and discharge to surface water via drainage systems. The FOOTPRINT Soil Type (FST) methodology developed in the EU project FOOTPRINT (Dubus et al., 2009) to define the bottom boundary condition (and drain spacing), which has been adopted in the Swedish spatial modelling tool MACRO-SE (Steffens et al., 2015), is promising in this respect.

The current descriptions of surface processes in the models requires further attention, including the temporal variation of soil properties, which govern the infiltration of water, including the effects of sub-critical soil water repellency and surface sealing. The mixing layer concept also needs further consideration. Tillage and traffic effects on macroporosity are currently not considered in the modelling. The temporal dynamics of ploughing should be included in future developments. Plough pans might be important and this also needs further attention. A harrowed layer is common in agricultural soils. A homogenized top layer is produced by seedbed preparation and will re-structure in due course. The temporal dynamics of this process needs further study. It would also be important to further investigate the temporal variation of biopore density, for example related to the re-colonisation of tilled layers by earthworms. Knowledge

of earthworm ecology could be useful to better understand the distribution of biopores in different soil horizons at the plot and field scale (van Schaik et al., 2010) and for contrasting soil types and land management practices at the larger landscape scale (Lindahl et al., 2009).

In the Netherlands there are initiatives to use MODFLOW and MT3D (ground water models). This may result in a better performance of the drainage models. Similar developments are planned in Denmark to link the output of the MACRO model to a groundwater model. In such approaches, it is very important to pay careful attention to the way the models are coupled, particularly when preferential flow is involved (Stenemo et al., 2005).

A strategy was proposed at the workshop for further model development. The first step consists of exploring potentially relevant processes that are not yet included in the models. In the next step, the model is adjusted and this is followed by field experimentation to test the improved models. It was stressed that reporting on exploring what turns out to be a non-sensitive or non-relevant process is important to ensure efficient model development.

Field experiments are also needed to understand scale-dependent processes (i.e. to generalize parameters obtained at small scales to larger scales). This is particularly important because field experiments are costly, so generic pedotransfer tools to estimate parameter values where no measurements are available are needed. There is also a need to identify ideal inert tracers or to identify a suitable tracer cocktail for field experiments.

At present there is no urgent need for new field studies. Instead, existing field studies which have not yet been exploited for model testing (i.e. the PLAP sites in Denmark), should be explored. It is recommended to test and compare the MACRO, PEARL-SWAP and HYDRUS models against such datasets. A working group (B. Jene, A. Rosenbom, S. Reichenberger and E. van den Berg) was set up to collate information on suitable datasets in Europe. A pan-european network of datasets would be helpful to ensure the best use of available data for further model testing and development. It was recommended to explore the possibilities for funding this work.

References

Armstrong, A., et al., 2000. Comparison of the performance of pesticide-leaching models on a cracking clay soil: results using the Brimstone Farm dataset. *Agricultural Water Management*, 44, 85-104

Abbaspour, K. C., A. Kohler, J. Šimůnek, M. Fritsch, and R. Schulín, Application of a two-dimensional model to simulate flow and transport in a macroporous agricultural soil with tile drains, *European Journal of Soil Science*, 52(3), 433-447, 2001.

Akay, O., G. A. Fox, and J. Šimůnek, Numerical simulation of water dynamics during macropore-subsurface drain interactions using HYDRUS, *Vadose Zone Journal*, 7(3), 909-918, 2008.

Alakukku, L., Nuutinen, V., Ketoja, E., Koivusalu, H., Paasinen-Kivekäs, M. 2010. Soil macroporosity in relation to subsurface drain location on a sloping clay field in humid climatic conditions. *Soil and Tillage Research*, 106, 275-284.

Assouline, S. 2004. Rainfall-induced soil surface sealing: a critical review of observations, conceptual models, and solutions. *Vadose Zone Journal*, 3, 570-591.

Beulke, S.; Brown, C. D.; Dubus, I. G.; Harris, G., 2001. Evaluation of uncalibrated preferential flow models against data for isoproturon movement to drains through a heavy clay soil. *Pest Management Science*, 57, 537-547.

Beven and Germann, 2013, Macropores and water flow in soils revisited. *Water Resources Research*, 49, 3071-3092.

Boivin, A., J. Šimůnek, M. Schiavon and M. Th. van Genuchten, Comparison of pesticide transport processes in three tile-drained field soils using Hydrus-2D, *Vadose Zone Journal*, 5(3), 838-849, 2006.

Cook, F. J., J. H. Knight, and R. A. Wooding, Steady groundwater flow to drains on sloping bed: Comparison of solutions based on Boussinesq equation and Richards equation, *Transport in Porous Media*, 77(3), 335-358, 2009.

Daniel, O., Kretzchmar, A., Capowicz, Y., Kohli, Y., Zeyer, J. 1997. Computer-assisted tomography of macroporosity and its application to study the activity of the earthworm *Aporrectodea nocturna*. *European Journal of Soil Science*, 48, 727-737.

Dubus, I., Brown, C.D. 2002. Sensitivity and first-step uncertainty analyses for the preferential flow model MACRO. *Journal of Environmental Quality*, 31, 227-240.

Dubus IG, Reichenberger S, Allier D, Azimonti G, Bach M, Barriuso E, Bidoglio G, Blenkinsop S, Boulahya F, Bouraoui F, Burton A, Centofanti T, Cerdan O, Coquet Y, Feisel B, Fialkiewicz W, Fowler H, Galimberti F, Green A, Grizzetti B, Højberg A, Hollis JM, Jarvis NJ, Kajewski I, Kjær J, Krasnicki S, Lewis KA, Lindahl A, Lobnik F, Lolos P, Mardhel V, Moeyers J, Mojon-Lumier F, Nolan BT, Rasmussen P,

Réal B, Šinkovec M, Stenemo F, Suhadolc M, Surdyk N, Tzilivakis J, Vaudour-Dupuis E, Vavoulidou-Theodorou E, Windhorst D, Wurm M, 2009. FOOTPRINT – Functional tools for pesticide risk assessment and management. Final report of the EU project FOOTPRINT (SSPI-CT-2005-022704), 221 p.

Dusek, J., Gerke, H. H., Vogel, T., 2008. Surface boundary conditions in two-dimensional dual-permeability modeling of tile drain bromide leaching. Vadose Zone Journal, 7, 1241-1255.

EFSA, 2013. Scientific Opinion on the report of the FOCUS groundwater working group (FOCUS, 2009): assessment of lower tiers. EFSA Journal, 11(2), 3114, 29 pp.

Ellerbrock, R. H., Gerke, H. H., 2013. Characterization of organic matter composition of soil and flow path surfaces based on physicochemical principles: a review. Advances in Agronomy 121, 117-177.

Ernst, L. F., Groundwaterstromingen in de verzadigde zone en hun berekening bij aanwezigheid van horizontale evenwijdige open leidngen (Groundwater flow in the saturated zone and its calculation when horizontal parallel open conduits are present), Versl. Landbouwk. Onderz. 67.1, Pudoc, Wageningen, 189 pp., the Netherlands (in Dutch), 1962.

Filipović, V., F. J. K. Mallmann, Y. Coquet, and J. Šimůnek, Numerical simulation of water flow in tile and mole drainage systems, Agricultural Water Management, 146, 105-114, 2014.

Flury, M. 1996. Experimental evidence of transport of pesticides through field soils – a review. Journal of Environmental Quality, 25, 25-45.

Gärdenäs, A., J. Šimůnek, N. Jarvis, and M. Th. van Genuchten, Two-dimensional modelling of preferential water flow and pesticide transport from a tile-drained field, Journal of Hydrology, 329, 647-660, 2006.

Gaur, A., Horton, R.; Jaynes, D. B.; Baker, J. L., 2006. Measured and predicted solute transport in a tile drained field. Soil Science Society of America Journal, 70, 872-881.

Gerke, H.H., van Genuchten, M.T., 1993a. A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media. Water Resources Research, 29, 305-319.,

Gerke, H.H., van Genuchten, M.T., 1993b. Evaluation of a first-order water transfer term for variably-saturated dual-porosity flow models. Water Resources Research, 29, 1225-1238.

Gerke, H.H., Köhne, J.M. 2002. Estimating hydraulic properties of soil aggregate skins from sorptivity and water retention. Soil Science Society of America Journal, 66, 26-36.

Gerke, H.H. Preferential flow descriptions for structured soils. Journal of Plant Nutrition and Soil Science, 169, 382-400, 2006

Gerke, H. H., Dusek, J., Vogel, T. and Kohne, J. M., 2007. Two-dimensional dual-permeability analyses of a bromide tracer experiment on a tile-drained field. *Vadose Zone Journal*, 6, 651-667.

Gerke, H. H., Dusek, J., and Vogel, T., 2013. Solute mass transfer effects in two-dimensional dual-permeability modeling of bromide leaching from a tile-drained field. *Vadose Zone Journal* 12, 91.

Germann, P.F. 1985. Kinematic wave approach to infiltration and drainage into and from soil macropores. *Trans. ASAE*, 28, 745-749.

Haarder, E. B., Looms, M. C., Jensen, K. H. and Nielsen, L., 2012. Visualizing unsaturated flow phenomena using high-resolution reflection ground penetrating radar. *Vadose Zone Journal*, 10, 84-97.

Haria, A.H., Johnson, A.C., Bell, J.P., Batchelor, C.H. 1994. Water-movement and isoprotruron behavior in a drained heavy clay soil. 1. Preferential flow processes. *Journal of Hydrology*, 163, 203-216.

Haws, N. W., P. S. C. Rao, J. Šimůnek, and I. C Poyer, Single-porosity and dual-porosity modeling of water flow and solute transport in subsurface-drained fields using effective field-scale parameters, *J. of Hydrology* , 313(3-4), 257-273, 2005.

Healy, R. W., *Simulating Water, Solute, and Heat Transport in the Subsurface with the VS2DI Software Package*, *Vadose Zone J.*, 7, 632-639, doi:10.2136/vzj2007.0075, 2008.

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

Heppell C.M., Burt T.P., Williams, R.J. 2000. Variations in the hydrology of an underdrained clay hillslope. *Journal of Hydrology*, 227, 236-256.

Hooghoudt, S. B., *Bijdrage tot de kennis van enigenatuutkundigegrootheden van de grond (Contribution to the knowledge of several physical soil parameters)*, *Versl. Landbouwk. Onderz.* 46 (14) B, 515-707, Wageningen, the Netherlands (in Dutch), 1940.

Hunt, A., Ewing, R., Ghanbarian, B. 2014. *Percolation theory for flow in porous media. Lecture Notes in Physics 880 (third edition)*. Springer-Heidelberg, 447 pp.

Jarvis, N.J., Jansson, P-E., Dik, P.E. and Messing, I. 1991. Modelling water and solute movement in macroporous soil. I. Description of the model and sensitivity analysis. *Journal of Soil Science*, 42, 59-70.

Jarvis, N.J. 1994. The MACRO model (Version 3.1). Technical description and sample simulations. Reports and dissertations 19, Department of Soil Science, Swedish Univ. Agric. Sci., 51pp.

Jarvis, N.J. 2007. Review of non-equilibrium water flow and solute transport in soil macropores: principles, controlling factors and consequences for water quality. *European Journal of Soil Science*, 58, 523-546.

Jarvis, N. J., Brown, C.D., Granitza, E., 2000. Sources of error in model predictions of pesticide leaching: a case study using the MACRO model. *Agricultural Water Management*, 44, 247-262.

Jarvis, N., Larsbo, M., Roulier, S., Lindahl, A. & Persson, L. 2007. The role of soil properties in regulating non-equilibrium macropore flow and solute transport in agricultural topsoils. *European Journal of Soil Science*, 58, 282-292.

Jarvis, N.J., Moeys, J., Hollis, J.M., Reichenberger, S., Lindahl, A.M.L. & Dubus, I.G. 2009. A conceptual model of soil susceptibility to macropore flow. *Vadose Zone Journal*, 8, 902-910.

Jarvis, N.J., Moeys, J., Koestel, J., Hollis, J.M. 2012. Preferential flow in a pedological perspective. In: *Hydropedology: synergistic integration of soil science and hydrology* (ed. H. Lin), Academic Press, Elsevier B.V., pp.75-120.

Jury, W.A. and K. Roth. 1990. Transfer functions and solute movement through soil: Theory and application. Birkhäuser, Basel (Switzerland).

Kätterer, T., Schmied, B., Abbaspour, K.C., Schulin, R. 2001. Single- and dual-porosity modelling of multiple tracer transport through soil columns: effects of initial moisture and mode of application. *European Journal of Science*, 52, 25-36.

Kluitenberg, G.J., Horton, R. 1990. Effect of solute application method on preferential solute transport in soil. *Geoderma*, 46, 283-297.

Kneale, W.R. 1986. The hydrology of a sloping, structured clay soil at Wytham, near Oxford, England. *Journal of Hydrology*, 85, 1-14.

Köhne, J.. M. and H. H. Gerke, Spatial and temporal dynamics of preferential bromide movement towards a tile drain, *Vadose Zone Journal* , 4, 79-88, 2005.

Köhne, J.M., Gerke, H.H., Köhne, S. 2002. Effective diffusion coefficients of soil aggregates with surface skins. *Soil Science Society of America Journal*, 66, 1430-1438.

Köhne, J. M., S. Köhne, and J. Šimůnek, A review of model applications for structured soils: a) Water flow and tracer transport, *J. Contam. Hydrology*, Special Issue "Flow Domains", 104(1-4), 4-35, 2009a.

Köhne, J. M., S. Köhne, and J. Šimůnek, A review of model applications for structured soils: b) Pesticide transport, *J. Contam. Hydrology*, Special Issue "Flow Domains", 104(1-4), 36-60, 2009b.

Köhne, S., B. Lennartz, J. M. Köhne, and J. Šimůnek, Bromide transport at a tile-drained field site: experiment, and one- and two-dimensional equilibrium and non-equilibrium numerical modeling, *Journal of Hydrology*, 321(1-4), 390-408, 2006.

Larsbo, M., Jarvis, N.J. 2005. Simulating solute transport in a structured field soil: uncertainty in parameter identification and predictions. *Journal of Environmental Quality*, 34, 621-634.

Larsbo, M., Roulier, S., Stenemo, F., Kasteel, R. & Jarvis, N.J. 2005. An improved dual-permeability model of water flow and solute transport in the vadose zone. *Vadose Zone Journal*, 4, 398-406.

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

Leeds-Harrison, P.B., Spoor, G., Godwin, R.J. 1982. Water flow to mole drains. *Journal of Agricultural Engineering Research*, 27, 81-91.

Leeds-Harrison, P.B., Shipway, C.J.P., Jarvis, N.J., Youngs, E.G. 1986. The influence of soil macroporosity on water retention, transmission and drainage in a clay soil. *Soil Use and Management*, 2, 47-50.

Leij, F.J., Ghezzehei, T., Or, D. 2002. Analytical models for soil pore-size distribution after tillage. *Soil Science Society of America Journal*, 66, 1104-1114.

Leue, M., Gerke, H. H., Ellerbrock, R. H., 2013. Millimetre-scale distribution of organic matter composition at intact biopore and crack surfaces. *European Journal of Soil Science* 64, 6, 757-769.

Lindahl, A.M.L., Dubus, I.G. & Jarvis, N.J. 2009. A site classification scheme to predict the abundance of the deep-burrowing earthworm *Lumbricusterrestris* L. *Vadose Zone Journal*, 8, 911-915.

Messing, I., Jarvis, N.J. 1990. Seasonal variation in field-saturated hydraulic conductivity in two swelling clay soils in Sweden. *Journal of Soil Science*, 41, 229-237.

Messing, I., Jarvis, N.J. 1993. Temporal variation in the hydraulic conductivity of a tilled clay soil as measured by tension infiltrometers. *Journal of Soil Science*, 44, 11-24.

Mohanty, B. P., R. S. Bowman, J. M. H. Hendrickx, J. Šimůnek, and M. Th. van Genuchten, Preferential transport of nitrate to a tile drain in an intermittent-flood-irrigated field: Model development and experimental evaluation, *Water Resources Research*, 34(5), 1061-1076, 1998.

Nielsen, M. H., Styczen, M., Ernstsens, V., Petersen, C. T., Hansen, S., 2010. Field study of preferential flow pathways in and between drain trenches. *Vadose Zone Journal*, 9, 1073-1079.

Oberdorster, C., Vanderborght, J., Kemna, A., Vereecken, H., 2010. Investigating preferential flow processes in a forest soil using time domain reflectometry and electrical resistivity tomography. *Vadose Zone Journal*, 9, 350-361.

Pruess, K. 1991. TOUGH2: A general-purpose numerical simulator for multiphase fluid and heat flow. LBL-29400. Lawrence Berkeley Natl. Lab., Berkeley, CA.

Raats, P.A.C. 1981. Residence times of water and solutes within and below the root zone. *Agricultural Water Management*, 4, 63-82.

Ritzema, H. P., 1994. Subsurface flow to drains. *Drainage Principles and Applications*, ed. 2, 263-304.

Rosenbom, A. et al. 2009. Numerical analysis of water and solute transport in variably-saturated fractured clayey till. *J. Contam. Hydrol.*, 104, 137-152.

Schlüter, S., H.-J. Vogel, O. Ippisch, P. Bastian, K. Roth, H. Schelle, 2012. Virtual Soils: Assessment of the Effects of Soil Structure on the Hydraulic Behavior of Cultivated Soils. *Vadose Zone J.* 11: -. doi:10.2136/vzj2011.0174.

Schlüter, S., J. Vanderborght, H.J. Vogel. 2012. Hydraulic non-equilibrium during infiltration induced by structural connectivity. *Adv. Water Resour.* 44: 101-112. doi:10.1016/j.advwatres.2012.05.002.

Schwen A., Bodner, G., Scholl, P., Buchan, G.D., Loiskandl, W. 2011. Temporal dynamics of soil hydraulic properties and the water-conducting porosity under different tillage. *Soil and Tillage Research*, 113, 89-98.

Šimůnek, J., N. J. Jarvis, M. Th. van Genuchten, and A. Gärdenäs, Review and comparison of models for describing non-equilibrium and preferential flow and transport in the vadose zone, *Journal of Hydrology*, 272, 14-35, 2003.

Šimůnek, J. and M. Th. van Genuchten, 2008. Modeling nonequilibrium flow and transport with HYDRUS, Special Issue "Vadose Zone Modeling", *Vadose Zone Journal*, 7(2), 782-797, 2008.

Šimůnek, J., M. Th. van Genuchten, and M. Šejna, Development and applications of the HYDRUS and STANMOD software packages and related codes, *Vadose Zone Journal*, doi:10.2136/VZJ2007.0077, Special Issue "Vadose Zone Modeling", 7(2), 587-600, 2008.

Soll, W., Birdsell, K. 1998. The influence of coatings and fills on flow in fractured, unsaturated tuff porous media systems. *Water Resources Research*, 34, 193-202.

Stamm, C., Sermet, R., Leuenberger, J., Wunderli, H., Wydler, H., Flühler, H., Gehre, M. 2002. Multiple tracing of fast solute transport in a drained grassland soil. *Geoderma*, 109, 245-268.

Steffens, K.; Larsbo, M.; Moeys, J.; Jarvis, N.; Lewan, E., 2013. Predicting pesticide leaching under climate change: importance of model structure and parameter uncertainty. *Agriculture, Ecosystems & Environment*, 172, 24-34.

Steffens, K., Larsbo, M., Moeys, J., Kjellstrom, E., Jarvis, N., Lewan, E., 2014. Modelling pesticide leaching under climate change: parameter vs. climate input uncertainty. *Hydrology and Earth System Sciences*, 18, 479-491.

Steffens, K., Jarvis, N.J., Lewan, E., Lindström, B., Kreuger, J., Kjellström, E. & Moeys, J. 2015. Direct and indirect effects of climate change on herbicide leaching – a regional scale assessment in Sweden. *Science of the Total Environment*, 514, 239-249.

Stehouwer, R.C., Dick, W.A., Traina, S.J. 1993. Characteristics of earthworm burrow lining affecting atrazine sorption. *Journal of Environmental Quality*, 22, 181-185.

Stenemo, F., Jørgensen, P., Jarvis, N.J., 2005. Linking a one-dimensional pesticide fate model to a three-dimensional groundwater model to simulate pollution risks of shallow and deep groundwater underlying fractured till. *Journal of Contaminant Hydrology*, 79, 89-106.

Surdyk, N. et al. 2007. In: del Re, Capri, E., Fragkoulis, G., Trevisan M. (eds.), 'Environmental fate and ecological effects of pesticides', pp. 452-459. (D5)

Tiktak A, Hendriks R.F.A., Boesten J.J.T.I. (2012). Simulation of pesticide leaching towards surface water in a pipe-drained clay soil in the soil in the Netherlands. *Pest. Manag. Sci.* 68: 290-302.

Tiktak, A. R.F.A. Hendriks, J.J.T.I. Boesten, A.M.A. van der Linden, 2012. A spatially distributed model of pesticide movement in Dutch macroporous soils. *J. Hydrol.* 470-471, 361-327.

Trafford, B.D., Rycroft, D.W. 1973. Observations of the soil water regimes in a drained clay soil. *Journal of Soil Science*, 24, 380-391.

Utermann, J.; Kladvko, E. J.; Jury, W. A., 1990. Evaluating pesticide migration in tile-drained soils with a transfer function model. *Journal of Environmental Quality*, 19, 707-714.

Vanderborght, J. and Vereecken H., 2007. Review of dispersivities for transport modelling in soils. *Vadose Zone Journal*, 6, 29–52.

Van Dam, J. C., Groenendijk, P., Hendriks, R. F. A., Kroes, J. G., 2008. Advances of modeling water flow in variably saturated soils with SWAP. *Vadose Zone Journal*, 7, 640-653.

Van Schaik N.L.M.B., Hendriks R.F.A. and van Dam J.C., 2010. Parameterization of macropore flow using dye-tracer infiltration patterns in the SWAP model. *Vadose Zone Journal* 9, 95–106.

Van Schaik, L.; Palm, J.; Klaus, J.; Zehe, E.; Schroder, B., 2014. Linking spatial earthworm distribution to macropore numbers and hydrological effectiveness. *Ecohydrology*, 7, 401-408.



Vogel, H. J.; Cousin, I.; Ippisch, O.; Bastian, P., 2006, The dominant role of structure for solute transport in soil: experimental evidence and modelling of structure and transport in a field experiment. *Hydrology and Earth System Sciences*, 10, 495-506.

Youngs, E.G. 1976. Determination of the variation of hydraulic conductivity with depth in drained lands and the design of drainage installations. *Agricultural Water Management*, 1, 57-66.

Youngs, E.G. 1980. The analysis of groundwater seepage in heterogeneous aquifers. *Hydrological Sciences Bulletin*, 25, 155-165.

Appendix 1 Programme workshop

Thursday 23 October

- | | |
|------------------------|--|
| 14h00 – 14h05 | Welcome by Organizing Committee (Erik van den Berg) Information by local organizers (Michael Stemmer) |
| 14h05 – 14h20 | Introduction of participants |
| First session: | Workshop target and key-note speakers (Chair: Nick Jarvis) |
| 14h20 – 14h50 | Modelling drainage in macroporous soils J. Simunek (University of California Riverside, USA) |
| 14h50 – 15h20 | Multidimensional flow and drainage in macroporous soils: a state of the art. J. Vanderborght (Forschungszentrum Jülich, Germany) |
| Second session: | Model testing of current model concepts (Chair: Klaus Hammel) |
| 15h30 – 16h30 | Contributions by workshop participants on subtopic “ <i>Model testing for current model concepts</i> ” ; 10 min presentations + 5 min questions <ul style="list-style-type: none"> • Horst Gerke (ZALF): Characterization of intact biopore walls and aggregate coatings for describing local non-equilibrium and inter-domain mass transfer • Loes van Schaik (Uni-Potsdam): Biopores: earthworm influence on soil hydrology and drainage • Anette Rosenbom (GEUS): Can MACRO describe drainage at arable PLAP-fields during unsaturated conditions and snow melt? |
| 16h30 – 17h30 | Breakout discussion groups Introduction: Erik van den Berg <ul style="list-style-type: none"> • Group A : Process description of macropore flow and analysis of model concepts • Group B : Field and lab experiments for improvement of validation status |
| 17h45 – 18h45 | Breakout discussion groups A and B (continued) |
| 18h45 – 19h00 | Summary of breakout sessions A and B (Session group leaders) |
| 19h30 | Workshop dinner |

Friday 24 October

8h45 – 9h00

Summary of day 1 and program of day 2
Nick Jarvis and Erik van den Berg

Third session:

Model improvements and future testing

Chair: Bernd Gottesbüren

9h00 – 10h00

Contributions by workshop participants on subtopic "*Model improvement*"; 10 min presentations + 5 min questions

- N. Jarvis (SLU) , MACRO: current limitations and future developments:
- Christian Stamm (EAWAG): What are appropriate upper boundary conditions for modelling preferential flow in the Swiss Plateau?
- R. Hendriks (Alterra) , SWAP: current limitations and future developments
- Aaldrik Tiktak (PBL): A spatially-distributed model of pesticide movement in macroporous soils

10h30 – 12h30

Breakout discussion groups C and D
Introduction : Anton Poot

- Group C : Recommendations for improvement of model concepts
- Group D : Recommendations for field and lab experiments for improved models

12h30 – 12h45

Summary of breakout sessions C and D
(Session group leaders)

12h45 – 13h30

Lunch

13h30 – 15h30

General discussion of results of breakout sessions A to D
(Chair: Erik van den Berg)

15h30 – 16h00

Summary of workshop results and follow-up of workshop
Erik van den Berg

- Summary report
- Presentation
- Paper

Appendix 2 List of participants

| First Name | Surname | Affiliation | Type | Country |
|-------------|---------------|-----------------------------------|------------|---------|
| Arnaud | Boivin | ANSES | Regulator | FR |
| Horst | Gerke | ZALF Muncheberg | Research | GE |
| Anne Louise | Gimsing | Danish EPA | Regulator | DK |
| Bernd | Gottesbüren | BASF | Industry | GE |
| Klaus | Hammel | Bayer CropScience | Industry | GE |
| Rob | Hendriks | Alterra | Research | NL |
| Nick | Jarvis | SLU | Research | SE |
| Bernhard | Jene | BASF | Industry | GE |
| Max | Köhne | Helmholtz UFZ | Research | GE |
| Wolfram | König | UBA | Regulator | GE |
| Chris | Lythgo | EFSA | Regulator | EU |
| David | Patterson | Syngenta | Industry | UK |
| Anton | Poot | Ctgb | Regulator | NL |
| Wolfgang | Reiher | Knoell Consult | Consultant | FR |
| Stephan | Reichenberger | FOOTWAYS | Consultant | FR |
| Anette | Rosenbom | GEUS | Research | DK |
| Stephanie | Roulier | Makhteshim-Agan Europe | Industry | FR |
| Stephan | Schubert | DAS | Industry | GE |
| Andreas | Schwen | Vienna | Research | AU |
| Jirka | Simunek | Univ. California, Riverside | Research | USA |
| Christian | Stamm | Zurich, EAWAG | Research | CH |
| Michael | Stemmer | AGES | Regulator | AU |
| Aaldrik | Tiktak | PBL | Research | NL |
| Erik | Van den Berg | Alterra | Research | NL |
| Loes | van Schaik | Univ. Potsdam | Research | GE |
| Jan | Vanderborght | Forschungszentrum Jülich | Research | GE |
| Erwin | Zehe | Karlsruhe Institute of Technology | Research | GE |