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Concepts and dimensionality in modeling unsaturated water flow and solute transport

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Abstract

Many environmental studies require accurate simulation of water and solute fluxes in the unsaturated zone. This paper evaluates one- and multi-dimensional approaches for soil water flow as well as different spreading mechanisms to model solute behavior at different scales. For quantification of soil water fluxes, Richards' equation has become the standard. Although current numerical codes show perfect water balances, the calculated soil water fluxes in case of head boundary conditions may depend largely on the method used for spatial averaging of the hydraulic conductivity. Atmospheric boundary conditions, especially in the case of phreatic groundwater levels fluctuating above and below a soil surface, require sophisticated solutions to ensure convergence. Concepts for flow in soils with macropores and unstable wetting fronts are still in development. One-dimensional flow models are formulated to work with lumped parameters in order to account for the soil heterogeneity and preferential flow. They can be used at temporal and spatial scales that are of interest to water managers and policymakers. Multi-dimensional flow models are hampered by data and computation requirements. Their main strength is detailed analysis of typical multi-dimensional flow problems, including soil heterogeneity and preferential flow.

Three physically based solute-transport concepts have been proposed to describe solute spreading during unsaturated flow: The stochastic-convective model (SCM), the convection-dispersion equation (CDE), and the fractional advection-dispersion equation (FADE). A less physical concept is the continuous-time random-walk process (CTRW). Of these, the SCM and the CDE are well established, and their strengths and weaknesses are identified. The FADE and the CTRW are more recent, and only a tentative strength–weakness–opportunity–threat (SWOT) analysis can be presented at this time. We discuss the effect of the number of dimensions in a numerical model and the spacing between model nodes on solute spreading and the values of the solute-spreading parameters.

In order to meet the increasing complexity of environmental problems, two approaches of model combination are used: Model integration and model coupling. A main drawback of model integration is the complexity of the resulting code. Model coupling requires a systematic physical domain and model communication analysis. The setup and maintenance of a hydrologic framework for model coupling requires

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substantial resources, but on the other hand, contributions can be made by many research groups.

Keywords: Vadose zone; Richards' equation; simulation; macropores; unstable wetting fronts; dispersion; FADE; random walk; model coupling; framework

Introduction

Knowledge about water flow and solute transport in the unsaturated zone is important for many environmental studies, such as:

- irrigation and drainage strategies (efficient water use);
- uptake of water and nutrients by crops (agronomic interest);
- transport of nutrients and pesticides towards groundwater and surface-water systems (pollution);
- management of salinity in irrigated agriculture (sustainability);
- surface-water management of agricultural and natural areas (agronomic and ecological interest).

The objective of this paper is to describe and evaluate current concepts for modeling of water flow and solute transport in the unsaturated zone. The main focus is the use of Richards' equation for soil water flow and on solute-spreading mechanisms in one or more dimensions. Model integration or model coupling of water flow and solute transport models is increasingly used to address complex environmental problems. In the final part of the paper we present a SWOT (Strengths, Weaknesses, Opportunities and Threats) analysis pertaining to these approaches.

Water flow

Soil water flow equations

The simplest types of soil water flow models act as tipping buckets. They ignore the vertical soil moisture gradient within the root zone, and losses by evaporation, transpiration and percolation are a function of the average degree of saturation of the root zone. Capillary rise can only be included in very simple ways. Well-known examples were provided by Deardorff (1978) for climate modeling, Smith (1992) and Allen et al. (1998) for irrigation scheduling, and Laio et al. (2001) and Guswa, Celia, and Rodriguez-Iturbe (2002) for ecohydrological modeling. In general the soil water fluxes calculated by tipping-bucket models are not accurate enough to quantify solute transport. Darcy's law has been accepted by most soil physicists for quantification of soil water fluxes in a continuum of soil, air and water at the scale of a representative elementary volume, often termed REV. The Richards' equation is based solely on Darcy's law and the continuity equation. Therefore it is strongly physically based, generally applicable, and can be used for fundamental research and scenario analysis. For variably saturated, rigid, isothermal porous media with incompressible water and a continuous air phase, Richards' equation extended with root water uptake can be written as:

$$\frac{\partial \theta}{\partial t} = C(h)\frac{\partial h}{\partial t} = \nabla \cdot \left[\mathbf{K}(h) \nabla h \right] - \frac{\partial K_z(h)}{\partial z} - S(h) \tag{1}$$

where θ is the volumetric water content (L^3L^{-3}), h is the pressure head (L), C is the differential moisture capacity $\partial\theta/\partial h$ (L^{-1}), t is the time (T), $\mathbf{K}$ is the hydraulic conductivity tensor (LT^{-1}) with K_z the hydraulic conductivity in the z direction, z is the

vertical co-ordinate (positive upward) (L), and S is a sink term for root water extraction ($L^3L^{-3}T^{-1}$).

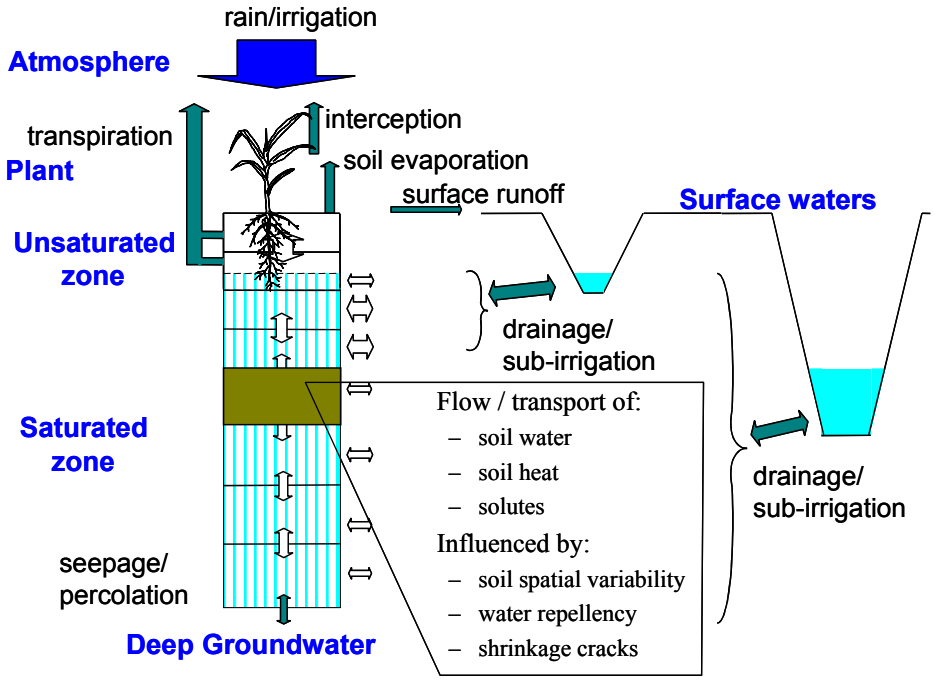

Figure 1. Schematization of hydrological processes incorporated in SWAP

Numerical discretization

Equation (1) is a partial differential equation which is highly non-linear due to the non-linear physical relationships between θ-h-K. Moreover at the soil surface, boundary conditions change rapidly and irregularly. Therefore, Richards' equation can be solved analytically only for a very limited number of cases. If the relationships between θ-h-K are known, numerical methods may solve soil water movement in top soils for any boundary condition. Several numerical techniques for one and more dimensions have been described by Yeh (1999) and Nieber and Feddes (1999).

In the past, many numerical schemes resulted in serious errors in the water balance due to the non-linearity of the differential moisture capacity C. An important step forward was made with the so-called mixed scheme, as proposed by Milly (1984) and Celia, Bouloutas and Zarba (1990). They eliminated elegantly the differential moisture capacity by using effectively the predicted soil water pressure heads of the former iteration step. Such mixed schemes show accurate water balances. However, the results of current numerical soil water flow models may be seriously affected by the way they average the hydraulic conductivity K between nodes. Haverkamp and Vauclin (1979), Belmans, Wesseling and Feddes (1983) and Hornung and Messing (1983) proposed to use the geometric mean, which increased the accuracy of calculated fluxes and caused the fluxes to be less sensitive to changes in nodal distance. However, the geometric mean has serious disadvantages too. When simulating infiltration in dry soils or high evaporation from wet soils, the geometric mean severely underestimates the water fluxes (1991) and may cause convergence problems of the iterative scheme due to steepening of the wetting front (Zaidel and Russo 1992). Other researchers viewed the soil hydraulic resistance as composed of a number of thinner resistances in series and proposed the use of a harmonic mean. Also, all kinds of spatial weighting schemes of K are used (Warrick 1991; Zaidel and Russo 1992; Desbarats 1995; Baker 1995; Romano, Brunone and Santini 1998; Gasto,

Grifoll and Cohen 2002; Brunone et al. 2003). The different approaches may have a significant effect on the calculated soil water fluxes, and many model users are not aware of this.

Van Dam and Feddes (2000) investigated the effect of nodal distance and averaging of hydraulic conductivity with SWAP (Soil–Water–Atmosphere–Plant). This model has been developed at Wageningen UR from 1978 onwards (Feddes, Kowalik and Zaradny 1978; Belmans, Wesseling and Feddes 1983; Kabat, Van den Broek and Feddes 1992; Van Dam et al. 1997; Kroes and Van Dam 2003) and simulates one-dimensional (1D), variably saturated, water flow, solute transport and heat flow in relation to crop development (Figure 1). One of the investigated cases concerned an intensive rain shower on a dry sandy soil. Van Dam and Feddes (2000) varied the nodal distance from 0.1 to 5 cm and applied both arithmetic and geometric averaging of K. At small nodal distances the hydraulic gradient and the average K converge to the same value, whatever method of K-averaging was used. Therefore a reference solution was derived with a nodal distance $\Delta z_i = 0.1$ cm. Figure 2 shows the simulated infiltration rate. For the reference case R, until $t = 0.008$ d, the hydraulic head gradient at the soil surface was large enough to absorb the high rain flux density of 1000 mm d^{-1}. At $t = 0.008$ d, h at the soil surface became zero. The infiltration rate declined and gradually approached the saturated hydraulic conductivity of 175 mm/d. The total amount of infiltration was 39 mm out of 100 mm of rainfall, the remaining amount was runoff. The use of arithmetic averages results in larger hydraulic conductivities and thus larger soil water fluxes than the use of geometric averages. Therefore in case of $\Delta z_i = 5$ cm, arithmetic averages of K overestimated the amount of infiltration (S3: 47 mm) while geometric averages seriously underestimated the amount of infiltration (S4: 27 mm). The very steep wetting front due to low geometric K averages caused infiltration rate oscillations at S2 and S4. These oscillations gradually decreased when smaller nodal distances were used, but convergence to the final solution was relatively slow (Figure 2). Harmonic means (not shown here) underestimated the mean K at the wetting front and the infiltration rate even more than the geometric mean. However, in case of arithmetic averages with $\Delta z_i = 1$ cm (S1), the calculated infiltration rate was close to that of the reference simulation R. Van Dam and Feddes (2000) showed similar results for soil evaporation cases. Both for extreme cases of infiltration and evaporation at soil textures ranging from sand to clay, nodal distances of 1 cm combined with arithmetic averaging of K yielded soil water fluxes that were close to the theoretical fluxes. Therefore in the 1D model SWAP variable node spacing (smaller spacing near soil surface and at extreme texture transitions) with arithmetic averaging of K is applied (Kroes and Van Dam 2003).

The above analysis supports the use of arithmetic averages in commonly applied finite-element numerical schemes (e.g. Šimůnek, Šejna and Van Genuchten 1998; 1999). However to avoid excessive calculation time in two-dimensional (2D) and three-dimensional (3D) problems, one tends to work with grid sizes much larger than 1 cm, especially in case of long-term periods, large flow domains and inverse problems. The larger grid sizes may significantly affect the calculated boundary fluxes, especially at the soil surface. For a reliable solution of these multi-dimensional problems, smaller grid sizes e.g. with adaptive grid refinement (Mansell et al. 2002) or specific weighting schemes (Brunone et al. 2003) seem indispensable.

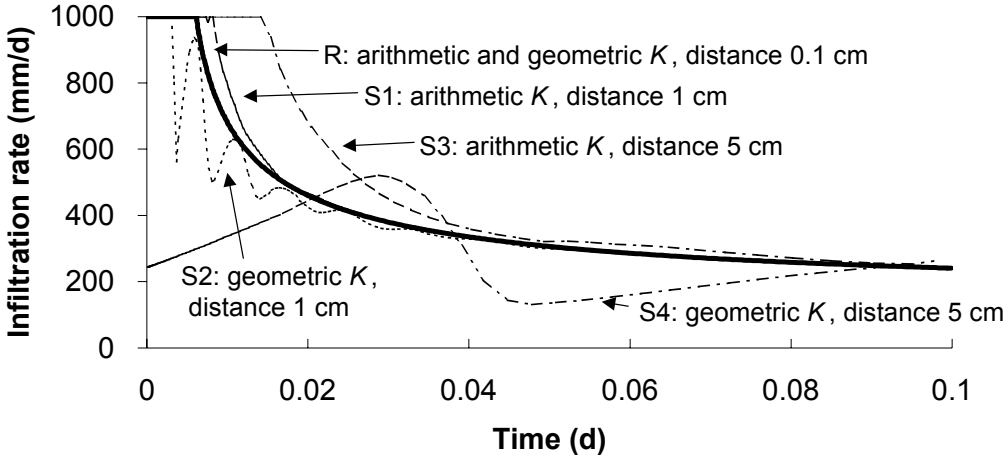

Figure 2. Simulated infiltration rate of sand during intensive rain (1000 mm d-1) after a dry period (θ_i i = 0.10) for different nodal distances and spatial averages of hydraulic conductivity K (S1-S4). The reference solution R was derived at a nodal distance of 0.1 cm for both arithmetic and geometric K averages

Boundary conditions

At the soil surface, the state variables may change rapidly by various orders of magnitude. For instance, after a few days with a relative air humidity of 50%, the soil water pressure head h will go down to -10^6 cm. At subsequent rainfall or irrigation with high but realistic intensities, in a few minutes h will become zero at the soil surface. At the same time the hydraulic conductivity K may increase with 5-8 orders of magnitude. In addition the relations between θ-h-K are highly non-linear. To simulate these infiltration events properly, extremely small time steps and strict convergence criteria for the numerical solution of Richards' equation are required.

Simulation of top boundary fluxes can also be problematic when groundwater levels fluctuate below and above soil surface, such as in polders and marsh lands. Especially after ponding conditions, when the soil profile becomes unsaturated, the soil water pressure head changes rapidly. Many current flow models which numerically solve Richards' equation do not reach convergence in such situations. Van Dam and Feddes (2000) developed a versatile procedure for 1D models that switches automatically from flux to head prescribed boundary conditions and vice versa, while solving Richards' equation accurately for conditions with shallow groundwater tables (Figure 3).

In 1D models, runoff is generally made equal to the amount of water exceeding a certain threshold for water ponding on the soil surface. With these models runoff along a slope can be analysed by treating the generated runoff at higher elevations as runon for lower elevations. In 2D and 3D models treatment of the runoff requires separate flow concepts like kinematic wave with proper surface resistances (Howes and Abrahams 2003).

Common lower boundary conditions in the soil are prescribed pressure heads h, soil water fluxes q, or relations between q and h. The latter relation is usually needed for scenario analysis. In case of deep groundwater levels free drainage conditions are generally applied. In case of shallow groundwater levels, drainage fluxes may consist of both local drainage and regional groundwater fluxes. The drainage fluxes can be determined by either simulating the 2D transect or by treating them as a sink in a 1D model (Figure 4). Accurate simulation of regional groundwater fluxes requires coupling of vadose zone models to groundwater flow models (see section on model coupling).

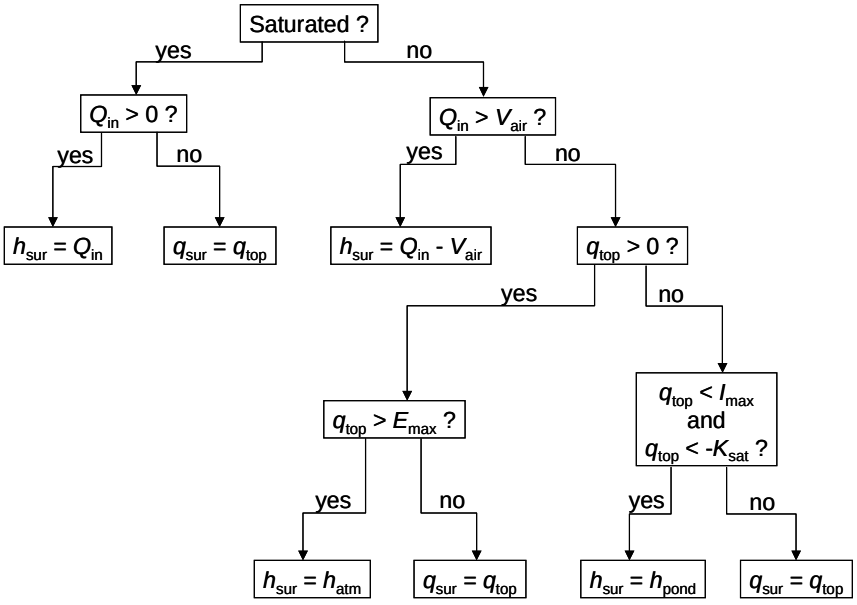

Figure 3. Procedure to select a head (h_{sur}) or flux (q_{sur}) top boundary condition (Van Dam and Feddes 2000). Q_{in} is the net water flow (L) into the soil column (including ponding water, root water extraction, drainage and seepage) during the time step, q_{top} (LT^{-1}) is the potential flux at the soil surface (positive upward), V_{air} (L) is the total air volume in the soil profile at the start of the time step, E_{max} (LT^{-1}) is the maximum soil evaporation, h_{atm} is the soil water pressure head in equilibrium with the air humidity, I_{max} (LT^{-1}) is the maximum soil infiltration, K_{sat} (LT^{-1}) is the top soil saturated hydraulic conductivity and h_{pond} (L) is the ponding height on the soil surface

Soil hydraulic functions

The soil hydraulic functions are fundamental to water and solute transport. There are many important reasons why analytical functions of $\theta(h)$ and $K(\theta)$ rather than tabulated data are used including the establishment of model databases, generation of scanning curves for hysteresis, convenient model input and parameter optimization. Van Genuchten (1980) described both $\theta(h)$ and $K(\theta)$ with only six parameters which are related to distinct soil physical properties. Significant deviations may occur near saturation for the $K(\theta)$ function (Vogel and Cislerova 1988; Durner 1994). A practical approach is to apply the analytical equations only to a certain unsaturated range (say h < -2 cm), and interpolate in the range near saturation (–2 < h < 0 cm) between the analytical functions and measured values of K at saturation (Vogel, Van Genuchten and Cislerova 2001).

Hysteresis of the $\theta(h)$ relation may complicate the measurement and use of the soil water characteristic. In the field wetting and drying occurs in numerous cycles, resulting in so-called drying and wetting scanning curves lying between the main drying and the main wetting curve. In practice, often only the main drying curve is used to describe the $\theta(h)$ relation. However, the simulation of infiltration events with the main drying curve can be misleading. Hysteresis will retard the infiltration front and increase runoff. A popular method to derive scanning curves is by rescaling the main wetting or the main drying curve to the actual water content (Scott, Farquhar and Kouwen 1983; Kool and Parker 1987). This method requires measurement of only the main wetting and drying curves. In order to avoid artificial pumping errors, Parker and Lenhard (1987) extended the scaling concept such that scanning loops always close. Among others, Lenhard, Parker and Kaluarachchi (1991), Dirksen et al. (1993) and Werner and Lockington

(2003) achieved good results with this hysteresis concept and consequently this concept has been adopted in many vadose zone models.

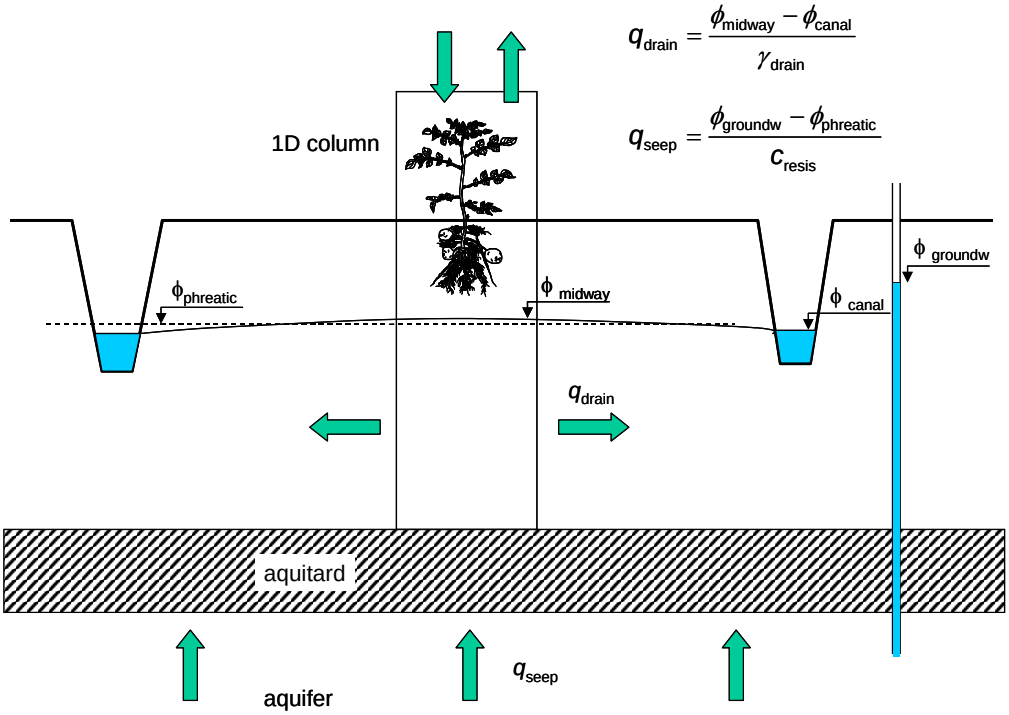

Figure 4. Superposition of local drainage fluxes and regional groundwater fluxes in SWAP. Here q_{drain} (LT^{-1}) is the drainage flux, q_{seep} (LT^{-1}) is the seepage flux from the first aquifer, ϕ_{midway}, $\phi_{phreatic}$, ϕ_{canal} and $\phi_{groundw}$ (L) are the hydraulic heads midway between the drains, mean of the phreatic aquifer, canal and first aquifer, respectively, γ_{drain} (T) is the drainage resistance and c_{resis} (T) is the resistance of the first aquitard. In the model q_{seep} is considered as bottom boundary condition, and q_{drain} as sink term in the Richards equation in the saturated part of the column

Databases which contain soil physical properties collected at a large number of laboratories (Leij et al. 1996; Wösten et al. 1999; 2001) can be used as direct model input, and are valuable to investigate the effects of soil hydraulic variability (e.g. Schaap and Leij 1998) and to derive versatile pedotransfer functions (Vereecken et al. 1989; Rawls, Ahuja and Brakensiek 1992; Van Genuchten et al. 1999; Wösten, Pachepsky and Rawls 2001). Innovative measurement techniques and efficient optimization algorithms create new opportunities to derive soil hydraulic functions by inverse modeling from laboratory and field experiments (Hopmans et al. 2002).

Spatial and time scale

Darcy's law (and consequently also Richards' equation) apply to an REV that can be viewed as a continuum of soil, water and air. In the case of soils with macropores or with unstable wetting fronts, such an REV does not exist for the entire soil matrix but does apply to different soil domains. In 3D models the specific soil physical properties of the different soil domains might be directly incorporated. In 1D and 2D models Richards' equation should be augmented with concepts that represent flow in the different domains. Šimůnek et al. (2003) provide a clear overview of non-equilibrium and preferential flow concepts for the vadose zone. In combination with these concepts, the spatial scale of Richards' equation might be increased to the field scale. This is very beneficial, as fields act as basic physical units of larger regions. Natural or

cultivated fields have predominantly one vegetation pattern, soil profile, drainage condition and management scheme. This information becomes increasingly accessible in geographical databases. Geographical information systems (GIS) can be used to generate input data for field scale models, to run these models for fields with unique boundary conditions and physical properties, and to compile regional results of viable water management scenarios. Recent examples of these studies are a national study (34,890 km^2) on the water-balance components of the hydrological top system in The Netherlands for nutrient management purposes (Kroes et al. 2002) and a water productivity analysis of irrigated crops in Sirsa district (4,100 km^2), India (Van Dam and Malik 2003).

The time scale for which Richards' equation is valid has no upper bound. This is very useful as hydrological conditions differ from year to year, while field experiments are mostly confined to a period of 1-3 years. In a field trial on pesticide leaching, Groen (1997) measured pesticide concentrations in drains which differed by 2-3 orders of magnitude between 2 successive years. Because of the year to year variability, pesticides in The Netherlands are evaluated with simulation models on their leaching potential in various soil types during a period of 70 years. It is important that extreme events during such a long period, especially those causing runoff and recharge, are handled properly without causing excessive calculation times. In case of 1D models this poses no problem. However, in case of 2D and 3D models a period of 70 years still requires substantial amounts of computation time. From 1960 onwards computation speed of personal computers has doubled each 1.5 year (Mansell et al. 2002). This means that simulations which nowadays require 1 hour, in 6 years may require less than 4 minutes. Therefore either time will solve this problem, or techniques such as parallel computing should be used.

Macropores

In structural biopores or macropores caused by swelling/shrinking or freezing/thawing, water flows much more quickly than through the soil matrix. Unfortunately, detailed simulation of physical transport processes in individual macropore networks is not feasible, as the chaotic and dynamic morphology of each location requires too many input data. Therefore one should search for some systematic behavior on a larger scale, in the same way as Darcy's law incorporates complicated, unpredictable pore geometry at the REV.

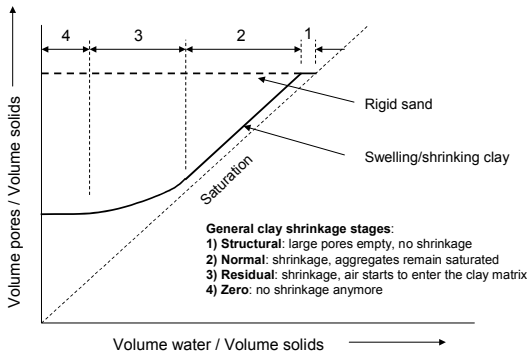

Figure 5. A clay shrinkage characteristic showing the four typical shrinkage stages

The MACRO model (Jarvis 1994; Larsbo and Jarvis 2003) is widely used to simulate water flow and solute transport in aggregated soils. In the MACRO model, two domains are distinguished, one with macropores and one with micropores. This is not a unique conceptualization and is commonly known as the dual-continuum or dual-porosity approach to simulate solute transport in macroporous soils. In the MACRO model, at the top boundary, the amount of water flowing into the macropore domain is simulated by an accurate solution of Richards' equation in the micropore domain, which generates the runoff. In the macropores, water flow is calculated by assuming a unit hydraulic gradient, equivalent to a kinematic wave approach. Water absorption from the macropore domain to the micropore domain is calculated with a diffusion equation. Gerke and Van Genuchten (1993) developed a dual-continuum model, in which Richards' equation is solved in both domains. One domain may represent the matrix and the other domain the macropores. The water exchange between the macropore and matrix at each node depends upon the pressure-head difference and a transfer coefficient. The soil physical properties of the macropore skin may differ from those of the bulk soil matrix, which hampers proper simulation of water exchange (Gerke and Köhne 2002). The relative volumes of matrix and macropores in the model of Gerke and Van Genuchten are assumed to be constant in depth and time and interaction with the groundwater is not possible.

In SWAP, the shrinkage characteristic is used to quantify the swelling and shrinking of a clay soil. Figure 5 shows a typical shrinkage characteristic, which relates the amount of water with the clay matrix volume (Stroosnijder 1976; Bronswijk 1988). The shrinkage characteristic can be used to calculate the crack volume and crack depth from the simulated water content in the clay matrix. Figure 6 shows the concept of water flow in a cracked clay soil as implemented in SWAP. Precipitation in excess of the infiltration rate flows as runoff to the cracks. Absorption of water flowing downward along the crack wall is not included. Bouma and Dekker (1978) and Booltink and Bouma (1993) concluded that the contact area between preferential flow and soil matrix is only a small fraction of the total vertical crack area and that the lateral absorption during flow along the crack walls can be neglected. Water collected at the bottom of the cracks may infiltrate laterally into the clay matrix or flow directly to drainage canals (Kroes and Van Dam 2003). Although the use of this concept considerably improves the calculation of water flow and solute transport in cracked clay soils, still deviations with reality exist. Simulations show more pronounced solute peaks than measured (Bronswijk, Hamminga and Oostindie 1995; Van Dam 2000). These differences are attributed to the use of one representative crack geometry. Probably important is the distribution of crack widths, orientations and depths, which cause water to infiltrate in the matrix at various depths (internal catchment). Hendriks, Oostindie and Hamminga (1999) distinguished a number of macropore domains, each with their own crack volume and depth, in order to simulate the internal catchment at various depths. However, with each additional macropore domain, the number of calibration parameters increases. Also Hendriks, Oostindie and Hamminga (1999) included static macropores which are always present, in addition to the dynamic macropores. These additions are currently being evaluated with SWAP for a number of field experiments (Hendriks 2003).

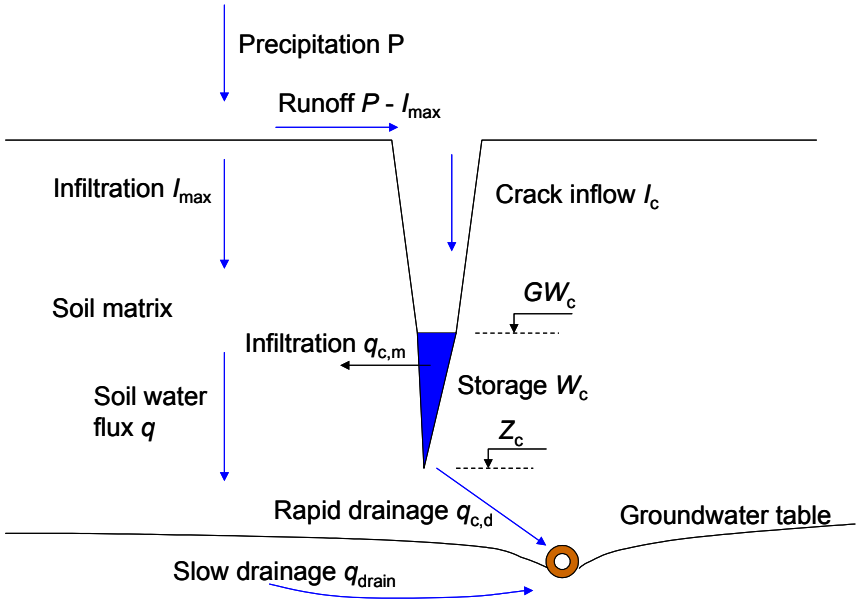

Figure 6. Concept of water flow in a cracked clay soil as applied in SWAP

Unstable wetting fronts

Preferential flow also occurs in seemingly uniform layered soils (e.g. De Rooij 2000). The most common factors are fine-textured layers overlaying more coarse-textured layers, air entrapment ahead of an infiltration front, and water repellency. In this section we will focus on water repellency. Water repellency is attributed to organic coatings of soil particles, to organic matter and to specific microflora. As a result of water repellency, water often flows through these soils in preferential flow paths or 'fingers', which affects transport of nutrients, salts and pesticides. Common approaches to simulate fingered flow by one-dimensional models are dual-porosity concepts (De Smedt and Wierenga 1979; Van Genuchten and Wagenet 1989; Gerke and Van Genuchten 1993; Saxena, Jarvis and Bergström 1994; Van Dam, Wösten and Nemes 1996; Elliot et al. 1998; Šimůnek et al. 2003). In case of dual-porosity models with one active flow domain, the volume of the active flow domain can be estimated by visual observation of dry and wet spots in the field shortly after precipitation, or more accurately with color tracer tests (Van Ommen et al. 1989; Flury and Flühler 1995), with a disc permeameter in combination with a tracer (Clothier, Kirkham and McLean 1992; Jaynes 2002), with TDR transect measurements of water content (Ritsema and Dekker 1994) or by model calibration (Van Dam et al. 1990; Šimůnek et al. 2003). Field observations show a time-dependent preferential flow path volume (Ritsema and Dekker 1994), which cannot be included in ordinary dual-porosity models. Also, dual-porosity models require typically twice as many soil physical parameters as single porosity models. Due to the difficulties to determine the parameter values by independent measurements, practical applications of dual-porosity models are still limited (Šimůnek et al. 2003).

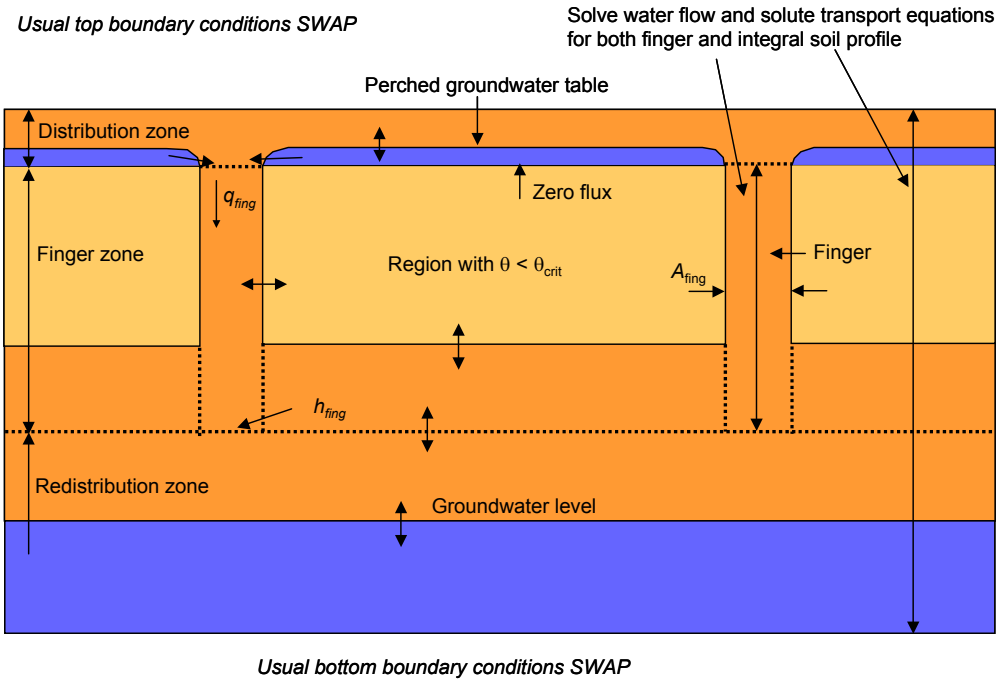

Figure 7. Extended concept of water flow in a soil profile with a water-repellent zone

One practical concept, which can be applied with readily available field data and accommodates the transient nature of preferential flow in water-repellent soils, is currently evaluated with SWAP. This concept is largely based on the work of Ritsema and Dekker (2000) and Selker, Steenhuis and Parlange (1996), and is illustrated in Figure 7. The soil profile contains a distribution zone where lateral flow may occur towards the fingers, a finger zone and a redistribution zone in which the fingers again merge. Fingers are formed when the water content below the distribution zone becomes smaller than a critical water content. Lateral diffusion of water from the fingers towards the surrounding water-repellent soil is neglected as it will be limited due to hysteresis and water repellency. The fingers will disappear if (1) due to evapotranspiration or percolation, the water content inside the fingers becomes less than the critical water content, (2) due to increasing groundwater levels or capillary rise, the water content below the distribution zone becomes larger than the critical water content, or (3) due to extreme fluxes in the top soil towards the fingers, the cross-sectional area of the fingers becomes too large. This flow concept enables simulation of the effects of water repellency on long-term water and solute balances and to analyse sensitivity to various physical factors (Ritsema et al. subm.; Kramers et al. in press).

Dimensionality

Soil processes have a three-dimensional character; modeling therefore, in principle, should employ three dimensions. However, important drawbacks of 3D models are the vast amount of input data, large computation times and laborious interpretation of results. Therefore, most current studies still employ 1D simulation models. Clearly, 1D models cannot reproduce reality, unless the soil profile is horizontally homogeneous and the boundary conditions are uniform. Examples where this may occur are laboratory set-ups with uniform soil cores, homogeneously layered lysimeters, or fields with deep groundwater levels and stable wetting fronts. To

overcome horizontal soil heterogeneities, either effective hydraulic properties of one domain or multi-domain concepts are often applied (Šimůnek et al. 2003).

An example of a 3D construct is flower cultivation on rockwool (Figure 8). In order to investigate the effect of physical properties of rockwool and fertigation strategies, a 3D model for water movement, solute transport, oxygen transport, root uptake of water and nutrients and root growth was developed (Heinen and De Willigen 2001). This model was coupled to a glasshouse crop model (Gijzen 1994).

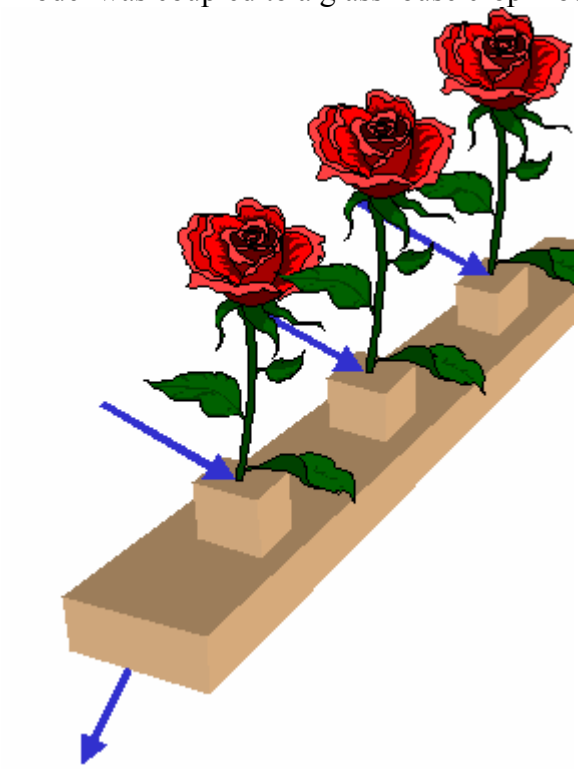

Figure 8. Example of a greenhouse growth system consisting of a rockwool slab with planting cubes. Water with dissolved nutrients is added by drip irrigation at the top of the planting cubes (arrows). Drainage may occur at one of the slab ends (arrow). The slope of the slab can be manipulated in any direction

When lines of symmetry are present, it is sometimes possible to consider flow in two dimensions only. Flow towards a single drain has been successfully modeled with a 2D transect model (De Vos 1997; De Vos, Hesterberg and Raats 2000; De Vos et al. 1999). The soil profile in de Vos' research was extremely layered and contained loose soil in the trench above the drain. By considering this specific heterogeneity in 2D, he was able to explain the observed fast leaching. By considering cylindrical axi-symmetry in a system, the 3D problem can be described by a 2D cylindrical model. This approach can be used for soil water flow surrounding single trees (Vrugt et al. 2001; Pronk, Heinen and Challa submitted).

The appropriate number of dimensions is closely related to the required accuracy of the research question. Therefore it is important that confidence intervals of model results be calculated.

SWOT analysis of one- and multi-dimensional models

Table 1 presents a SWOT analysis of one- and multi-dimensional models based on Richards' equation.

Table 1. SWOT analysis of one- and multi-dimensional soil water flow models based on Richards' equation

	One-dimensional model	Multi-dimensional model
Strength	▪ simplicity ▪ robust numerical scheme ▪ short calculation times ▪ availability of soil hydraulic data	▪ applies to unsaturated and saturated zone ▪ possibilities to consider effects of soil heterogeneity and preferential flow
Weakness	▪ only valid in unsaturated zone ▪ lumped parameters, which incorporate soil heterogeneity and preferential flow	▪ many input parameters are required ▪ computation times are large ▪ top boundary condition (correct Darcy flux; alternating ponding/dry)
Opportunity	▪ develop versatile flow concepts for soil heterogeneity and preferential flow at field scale level ▪ new field measurement techniques, remote sensing and efficient optimization routines facilitate calibration	▪ new techniques from numerical mathematics may increase stability of numerical solution ▪ parallel computers with adapted source code may decrease computation times
Threat	▪ unless sound techniques are developed for the interaction between top system and regional groundwater, the accuracy at regional scale will be problematic	▪ as multi-D models claim to consider (near) reality problems, modelers, engineers and policymakers may rely too much on the outcome: models will always remain an approximation of real soils

Main strengths of the 1D model are its simplicity and ability to solve Richards' equation accurately and efficiently. The vast amount of soil hydraulic data in accessible databases and the increasing accuracy of pedotransfer functions facilitate its application.

An important weakness is that in general 1D vertical flow is limited to the unsaturated zone. In the saturated zone water will flow according to the prevailing hydraulic head gradients in a 3D pattern. Another weakness concerns the lumped character of input parameters. These input parameters should incorporate 3D flow phenomena in the unsaturated zone.

However, 1D models also have a major opportunity to develop versatile flow concepts for soil heterogeneity and preferential flow. A few examples of these concepts for macroporous soils and water-repellent soils have already been discussed. These concepts can be applied to temporal and spatial scales that are of interest to managers and policymakers and are able to show the relevance of soil heterogeneity and preferential flow at these scales. Non-destructive and stand-alone field measurement techniques are increasingly becoming operational, such as remote sensing for soil surface wetness, surface temperature and evapotranspiration (Van Oevelen 2000; Bastiaanssen, Ahmad and Chemin 2002), scintillometers for evapotranspiration (Meijninger and De Bruin 2000), time-domain reflectrometry for water content (Ferre and Topp 2002), automatic sampling equipment for tracers (Groen 1997) and automatic groundwater level monitoring. The field data that these instruments provide allow automatic calibration of 1D models under natural conditions. Also, experiments that allow inverse modeling provide new opportunities to derive soil hydraulic functions economically (Hopmans et al. 2002). We may view fields with one vegetation pattern, soil profile, drainage condition and management scheme as natural basic units of larger regions. Within these units unsaturated flow is essentially one-dimensional. Consequently, 1D models in combination with

geographical information systems can be used to analyse water flow in the hydrological top system at the regional scale. However, recent regional studies show that the type of schematization significantly affects the lower boundary condition and the simulation results (Kroes et al. 2002; Tiktak, Van der Linden and Boesten 2003). Therefore more analysis is required to find reliable lower boundary conditions for these studies.

A major advantage of multi-dimensional models is that they apply to both the unsaturated and saturated zone. These models also provide excellent research opportunities to investigate effects of soil heterogeneity and preferential flow. It seems worthwhile to use these models to derive practical flow concepts that represent soil heterogeneity and preferential flow in 1D models.

Main weaknesses of 2D and 3D models are the requirement of vastly more input parameters and the long computation times, especially when dealing with regional studies, long-term simulations or inverse modeling problems. New numerical techniques, flexible parallel computing and faster computer processors will provide opportunities to diminish current long calculation times. The top boundary conditions require more attention. In case of head conditions at relatively dry or wet circumstances, the large nodal distances commonly used in 2D and 3D model result in inaccurate soil water fluxes. Also, alternating conditions of ponding and dryness, and non-homogeneous conditions at the soil surface, pose problems for current models.

A possible threat to 2D and 3D simulation models is their representation of reality, while they remain approximations of real soils. For instance, the amount of input data required will always remain a problem. This threat is weakened if operational numerical techniques are available to calculate confidence intervals of relevant model results.

Solute transport

Solute-spreading mechanisms

Three physically based mechanisms have been proposed to explain spreading of solutes as they travel through the soil with the moving liquid phase: travel-time variations within the population of stream tubes, the analogy with molecular diffusion, and Lévy processes (Table 2). Sorption and transformation processes can be equally well implemented in models based on any of these three spreading mechanisms. Other concepts have emerged, such as the mobile-immobile solute transport model (see Nielsen, Van Genuchten and Biggar (1986) for an overview of early work), but these are typically based on one of the three fundamental spreading mechanisms. For instance, some formulations of the mobile-immobile flow model assume the liquid phase in a soil to be partitioned in a mobile domain where flow occurs, and an immobile domain in which the soil solution is stagnant. Usually, the convection-dispersion equation (CDE) is valid in the mobile domain, and diffusion is assumed in the immobile domain (Van Genuchten and Wierenga 1976). A fourth mechanism has a less obvious physical connotation but merits attention because of its extraordinary generality: solute spreading by a continuous-time random-walk process (CTRW). CTRW describes solute movement in terms of the probability of a random displacement with a random travel time. It is distinct from random-walk models in which particle paths follow stream lines perturbed by random excursions (Berkowitz, Scher and Silliman 2000). This mechanism too can be implemented in derived modeling concepts, as was demonstrated by Dentz and Berkowitz (Dentz and Berkowitz 2003) who included CTRW in a mobile-immobile model.

Table 2. Solute-spreading mechanisms, with *N* the number of parameters required to describe solute spreading. The literature pertaining to the various models bases its terminology and acronyms on either 'convection' or 'advection'. We use these terms interchangeably here to conform to the adopted terminology

Spreading mechanism	Resulting solute-transport concept	*N*
Travel-time variation between stream tubes	Stochastic-convective model (SCM)	1
Analogy with molecular diffusion obeying Fick's law (Brownian motion)	Convection-dispersion equation (CDE)	1
Lévy process (Brownian motion interspersed with convective motion)	Fractional advection-dispersion equation (FADE)	2
Series of solute particle transitions	Continuous-time random walk (CTRW)	2

Conceptually the simplest of the four concepts in Table 2 is the stochastic-convective model (SCM): this modeling concept views a soil volume as a population of stream tubes with randomly distributed travel times. The travel-time probability distribution function (pdf) is often assumed to be lognormal (Jury 1982; Simmons 1982; Jury and Roth 1990), resulting in the convective lognormal transfer function model (CLT). In the SCM, solutes do not move with respect to the water which carries them: a solute particle never leaves the stream tube into which it entered at the inlet boundary of the soil volume, and at all times its velocity is equal to that of the water surrounding it (Figure 9). During stochastic-convective solute transport the degree of solute spreading in non-layered soils is proportional to the distance traveled, and the standard deviation of the travel time increases linearly with the travel distance (Jury and Roth 1990, eq. (2.70)). For steady-state flow, the standard deviation of the travel distance increases linearly with time. Because solute particles are assumed not to leave their stream tubes, the SCM can only model the longitudinal spreading within the entire soil volume and cannot handle non-uniform solute applications at the inlet boundary.

The solute transport concept implemented in most solute transport models is the convection-dispersion equation (CDE), which assumes a macroscopic uniform flow in which solutes are spread by a dispersive flux that is analogous to diffusion (i.e., proportional to the concentration gradient) and hence obeys Fick's law (Figure 9). The CDE reads:

$$\frac{\partial \theta c_l^r}{\partial t} = \nabla\left(\theta \mathbf{D} \nabla c_l^r\right) - \nabla\left(\mathbf{J}_w c_l^r\right). \tag{2}$$

Here, $\mathbf{D}$ (L^2T^{-1}) is a tensor consisting of effective dispersion coefficients, $\mathbf{J}_w$ is the vector of water flux densities (LT^{-1}) in the principal directions, c is the solute concentration (ML^{-3}), subscript l indicates the concentration relates to dissolved rather than sorbed solutes, and superscript r indicates a resident concentration (Parker and Van Genuchten 1984; Jury and Roth 1990, p. 45-53). The water flux densities in $\mathbf{J}_w$ are macroscopic, in the sense that local variations need not be explicitly accounted for. Instead, the effect these local variations in $\mathbf{J}_w$ have on solute spreading is reflected in the values of the elements of $\mathbf{D}$. For soils this means that soil layers are usually assumed to be uniform, resulting in essentially parallel, vertical flow lines for many applications. The tensor $\mathbf{D}$ is often simplified, with a scalar longitudinal dispersion coefficient (D_{long}) on the diagonal element corresponding to the axis parallel to the main flow direction, lateral (D_{lat}) dispersion coefficients (L^2T^{-1}) on the remaining

diagonal elements corresponding to the axes perpendicular to the main flow direction, and all off-diagonal elements equal to zero.

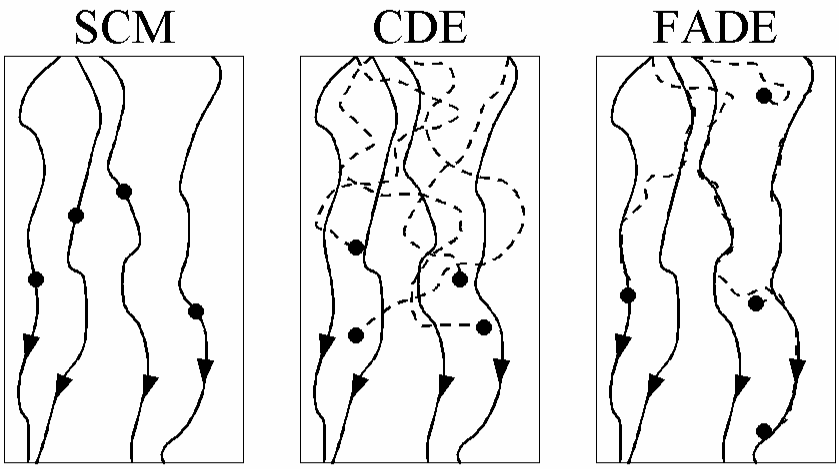

Figure 9. Three solute-spreading mechanisms in soil. The curved arrows indicate flow paths (solid lines), the black dots represent solute particles, and the dashed lines their trajectories. According to the stochastic-convective model (SCM), solutes remain within the flow tube in which they entered at the soil surface. The convection-dispersion equation (CDE) assumes solutes continuously change flow tubes through Brownian motion. The fractional advection-dispersion equation (FADE) allows for periods of Brownian motion interspersed with periods during which solute particles do not leave their flow tubes

The Fickian fluxes (represented by the second-order term in the right-hand side of Eq. (2)) cause solutes to spread in all directions. A mechanistic explanation of convective-dispersive solute transport invokes the assumption that solute particles randomly transfer among different stream tubes through Brownian motion, and by doing so experience a wide range of flow velocities (e.g. Flühler, Durner and Flury 1996). Given enough time, the distances negotiated by a solute particle in all principal directions with respect to the main direction of flow are composed of a large number of accumulated paths of varying length. Lyapunov's limit theorem (Harris and Stocker 1998, p. 801) stipulates that the longitudinal and lateral travel distances, and hence the locations, of a large number of solute particles that began their voyage at the same location at the same time should eventually become normally distributed. Indeed we find that the dispersive component of the solute flux for a solute released from an instantaneous point source in an infinite one-dimensional homogeneous medium results in a normally distributed solute distribution (e.g. Carslaw and Jaeger 1959, p. 50-51):

$$c_l^r\left(x_L,t\right)=\frac{1}{2\sqrt{\pi Dt}}\exp\left(\frac{-x_L^2}{4Dt}\right) \tag{3}$$

where x_L is the moving spatial co-ordinate (L) and D is the dispersion coefficient (L^2T^{-1}). In Eq. (3), $x_L = 0$ at the location of the plume center, which is determined by the convective travel distance since the time of solute application at $t = 0$. Equation (3) represents the normal distribution with zero mean and standard deviation $(2Dt)^{1/2}$ (compare Eq. (26) of Simmons 1982). The trend to normality of the concentration

distribution is fundamental to the CDE and is a direct consequence of the Fickian nature of the dispersive flux. For a pulsed solute application (uniform over the inlet boundary or as a point source), deviations from normality occur if the inlet boundary impairs solute movement out of the soil (e.g., at the soil surface). The Fickian dispersive fluxes in the direction of the boundary are obviously blocked, resulting in an asymmetrical solute plume. As the plume moves further into the soil, it will increasingly tend towards normality (Parker and Van Genuchten 1984).

Equation (3) implies that solute spreading in a uniform soil during steady-state flow is proportional to the square root of time. It follows that the standard deviation of the travel time during steady-state convective-dispersive solute transport in a uniform soil is proportional to the square root of the travel distance (Jury and Roth 1990, eq. (2.58)).

The fractional advection-dispersion equation (FADE) represents the intermediate stages between the SCM and the CDE and includes the CDE as a special case (Figure 9). While the development of the SCM was triggered by the inability of the CDE to reproduce field-scale solute leaching it was found that assuming no dispersion at all was too strict. For flow processes in other fields of physics, Fokker-Planck equations have been developed that use fractional derivatives to account for non-Brownian movements with long-range spatial dependence (memory effect) or high velocity variability (Benson, Wheatcraft and Meerschaert 2000b). In its simplest form (one-dimensional uniform flow, symmetric dispersion, uniform θ, conservative tracer), the fractional advection-dispersion equation is (Benson, Wheatcraft and Meerschaert 2000a; 2000b; Pachepsky, Benson and Rawls 2000):

$$\frac{\partial c_l^r}{\partial t} = \frac{D_f}{2}\left[\frac{\partial^\alpha c_l^r}{\partial x^\alpha} + \frac{\partial^\alpha c_l^r}{\partial(-x)^\alpha}\right] - \frac{J_w}{\theta}\frac{\partial c_l^r}{\partial x} \tag{4}$$

where x is the spatial co-ordinate (L), α is the order of the fractional derivative ($0 \le \alpha \le 2$), and the fractional dispersion coefficient D_f has dimensions $L^\alpha T^{-1}$. A comparison between Eqs. (2) and (4) immediately demonstrates their similarity. Equation (4) can be made considerably more flexible by adding a factor accounting for asymmetry (Benson, Wheatcraft and Meerschaert 2000a; Benson, Wheatcraft and Meerschaert 2000b).

Recently, continuous-time random-walk models (CTRW) (e.g. Berkowitz and Scher 1998) have been used in solute transport studies in saturated media. Such models retain the key features of space–time correlations of particles as they are convected across fractured networks of porous media over different spatial or temporal frames. Hence intermediate degrees of lateral mixing of solutes are permitted in CTRW, similar to the FADE. As solute transport is modeled with a series of 'particle transitions', the need to assume an average velocity (key to the CDE and the FADE) is removed.

For the SCM, the CDE and the FADE, the standard deviation of travel distance is proportional to powers of the mean travel time $\left(\Delta\bar{t}\right)^a$ and distance $\left(\Delta\overline{x_i}\right)^a$. The power a equals 1 for the SCM and 0.5 for the CDE. This implies solute spreading is considerably faster during stochastic-convective transport than it is during convective-dispersive transport. In the FADE, $a = \alpha^{-1}$ (Benson, Wheatcraft and Meerschaert 2000a). For $1 \le \alpha \le 2$, as appears to be common for soils (Pachepsky, Benson and Rawls 2000; Zhou and Selim 2003), the FADE is mathematically intermediate between the SCM and the CDE. Its physical basis is the Lévy process: A solute particle does not continuously wander between stream tubes, but experiences

convective episodes during which it remains in the same stream tube intermitted by Brownian, dispersive episodes (Pachepsky, Benson and Rawls 2000). Hence, the FADE is the intermediate between the SCM and the CDE in both a mathematical and a physical sense.

The CTRW model of Kosakowski, Berkowitz and Scher (2001) assumed a power-law dependence for the solute particle transitions over a distance x in a time t. In doing so, the parameter β, which is related to the medium dispersion, controls the nature of the solute transport. When β is greater than 2, the bulk solute travels with the mean water velocity in a Fickian manner consistent with the CDE; however, when β lies between 0 and 1, the solute plume scales to t^{β}, and when β is between 1 and 2, the solute plume moves with constant velocity, consistent with the SCM (Berkowitz, Scher and Silliman 2000; Berkowitz and Scher 2001). In this respect, both convective-dispersive and stochastic-convective flows can be modeled with CTRW and may be regarded as limiting cases of CTRW models.

CTRW models are different to FADE models; the former is dependent on β, a parameter related to the media dispersion; the latter dependent on α, a parameter related to the fractional order of differentiation. A comparison of these models was recently presented by Berkowitz et al. (2002), who demonstrated that fractional derivative formulations of temporal and spatial transport equations emerge as special cases of CTRW; however, more recently, Hilfer (2003) demonstrated that transport equations with fractional derivatives are not in general asymptotically equivalent to CTRW models.

Vanderborght et al. (2001) investigated whether the solute-spreading regime during leaching experiments in seven soils was convective-dispersive or stochastic-convective. They found that the occurrence of lateral impeding layers or narrow horizontal bands of contrasting texture could enhance lateral mixing, and thus promote convective-dispersive transport. Vertical conductive features (e.g., macropores, wet fingers) favored stochastic-convective transport; the relations between soil morphology and solute transport were somewhat ambiguous though. Vanderborght et al. based their analysis on the evolution with travel time or distance of D_{long}, which theoretically is constant for the CDE and linearly increases for the SCM. Both convective-dispersive and stochastic-convective transport were observed, sometimes even in the same soil, depending on the flow rate. The FADE and the CTRW were not included in the analysis, although the authors acknowledge the limitations of considering only two extreme solute-spreading mechanisms.

Effects of dimensionality and nodal density on solute spreading

In two- and three-dimensional numerical soil models in which soil heterogeneity is represented by some type of random variation of the nodal soil hydraulic properties, variations in convective travel times cause spatial and temporal solute spreading (termed convective solute spreading below), even when the macroscopic flow (averaged over many flow tubes) is unidirectional. This convective spreading is absent in multidimensional models in which soil layers are considered uniform and in one-dimensional models. The solute-spreading mechanism implemented in the model determines if and to what degree additional solute spreading occurs (termed dispersive solute spreading). It must be noted that SCM, CDE and FADE are used outside their appropriate range when solute spreading in a soil profile is modeled while heterogeneities within the decimeter scale are explicitly accounted for. These solute transport-modeling concepts were designed to model both convective and dispersive solute spreading as a result of any process that operates at a scale smaller than that of

the macroscopic flow pattern and lump these processes into a simple parameterization. The macroscopic flow pattern can be defined as the flow that would occur in the same domain under the same initial and boundary conditions, but for a soil with uniform layers. When small-scale heterogeneities are included in the water flow model, the convective part of the solute spreading is (partially) reproduced by the resulting variation in travel times and geometry of the water flow paths and the solute-spreading parameters should have smaller values to reflect their reduced contribution to the total solute spreading. In soils with marked heterogeneities not caused by random variations of the soil hydraulic properties of the matrix (e.g., flow through macropores or fingers), additional measures are required to model solute travel-time variations (see the discussion of two-domain models in the section on water flow).

In addition, the nature of the solute-spreading process changes with scale; at a given scale, the largest heterogeneities most strongly affect solute spreading (e.g., root holes in sampling cylinders and clay lenses in aquifers). Soil heterogeneity is therefore increasingly dominant over diffusion and pore scale dispersion at increasing scales (although diffusion may still be important during dry spells with negligible convective transport). At scales closely approximating a soil's REV (e.g., a laboratory column) the solute-spreading mechanism may be much better approximated by the Fickian dispersion flux of the CDE than it is at the plot and field scale (Simmons 1982).

Representing soil heterogeneity by nodal variations in soil hydraulic parameters has another effect: solute-spreading parameters in multidimensional numerical models become dependent on both the model discretization and the spatial detail of the soil hydraulic-properties data, and cannot automatically be carried over to other discretizations, or be compared with those of other soils. Determining the solute-spreading parameter values in such models becomes particularly complicated when the model employs a numerical discretization with widely varying nodal spacing. In such cases it is recommendable to represent soil heterogeneity at the most suitable nodal spacing only, which is determined from the level of spatial detail in the data and the method used to describe the soil's spatial variation. In model regions where the flow conditions would allow a larger nodal spacing, the penalty for doing so is an artificial reduction of the soil heterogeneity; in that case the minimal nodal density should be chosen such that a proper spatial structure of the numerical representation of the soil is preserved. In cases where the numerical solution requires a denser grid (e.g., near the soil surface and around drains, ditches or emitters), the soil hydraulic properties should not be allowed to vary randomly at scales below that at which the heterogeneity is characterized from data. If one does, one in fact extrapolates the variogram beyond its range of validity. Subgrid variations are represented by the variogram nugget, which, in most cases, would have taken a smaller value if data were obtained at smaller spatial intervals. Maintaining the same nodal spacing in representing the random component of spatial variability anywhere in the flow domain eliminates the need to adjust solute-spreading parameters to variations in nodal spacing in different model regions.

In numerical models that account for soil heterogeneity, the choice of the solute transport model needed to describe the dispersive solute spreading is less crucial than in models with macroscopic water flow, since convective solute spreading is already included. The SCM assumes all solute spreading to arise from random (stochastic) convective travel-time variations within a given soil volume. In the early literature (Jury, Stolzy and Shouse 1982), this soil volume represented an entire field, but the

concept is valid for smaller soil volumes as long as they are much larger than the pore size. In addition, the dimensions of the soil volume must be large in comparison to the cross-sectional area of the flow tubes intercepted by individual solute sampling devices. A convenient, albeit somewhat arbitrary, minimal volume for which the SCM is still valid would be a soil block in the order of one cubic meter (i.e., plot size). The nodal spacing of many numerical models nowadays is at least one or two orders of magnitude smaller than the size of such a block (resulting in thousands to millions of nodes in the block). Within the framework of a detailed soil model, we therefore can tacitly interpret the stochastic nature of the travel times central to the SCM as being determined deterministically from the random variations of the soil hydraulic properties. The SCM assumes no additional solute spreading; the spreading caused by the randomness of the soil hydraulic properties suffices.

The CDE assumes Fickian solute spreading. As was stated previously, this assumption may be acceptable on the laboratory column scale but not on the field scale (Simmons 1982). This seems to imply that using the CDE in a multidimensional model can work on the field scale if the nodal spacing is comparable to the laboratory column size (in the order of 0.1 m), provided that the variability of the soil hydraulic properties assigned to the individual nodes produces an adequate variation in the solute travel times of individual stream tubes. For large travel distances D_{long} and D_{lat} are frequently made proportional to the travel distance in the CDE to counter the CDE's tendency to underestimate solute spreading (e.g. Butters and Jury 1989). When the soil model includes heterogeneity, D_{long} and D_{lat} should remain constant, since the convective solute spreading should enhance the degree of solute spreading. Thus, large-scale solute spreading is dominated by convective variation, and small-scale spreading by Fickian dispersion. Consequently, applying the CDE in this manner effectively results in a model that can be considered a hybrid of the SCM and the CDE. It must be noted that the numerical model must adequately reproduce the occurrence of preferential flow paths in the field. With limited spatial dependence in the soil properties (no preferential flow paths), solute motions will become Brownian again on a sufficiently large scale.

The FADE is based on solute motions that are partially non-Brownian and have some memory effect. Its fractional derivatives can incorporate the effect of elongated areas of rapid solute movement (e.g., in preferential flow paths) that are unlikely to be represented by randomly varying soil hydraulic properties unless considerable spatial correlation is allowed in the main direction of flow. So far, the FADE has only been applied to one-dimensional problems. Meerschaert, Benson and Bäumer (1999) derived an expression for multidirectional fractional derivatives. Their use has not yet been demonstrated in multidimensional solute transport problems.

Reducing three-dimensional flow to a one-dimensional simplification

There are many valid reasons to choose a one-dimensional rather than a three-dimensional model, and these benefits can often be quantified in terms of computational effort, amount of pre- and post-processing, and data requirement. In order to make a well-founded choice between 1D and 3D models, it would be beneficial if the simplification of the solute transport process (the cost of opting for a 1D model) could be equally well quantified. The recently introduced leaching-surface concept (De Rooij and Stagnitti 2002b; 2002a) offers a tool to do so. The leaching surface is a curved surface that represents the temporal and spatial aspects of solute leaching at a given depth, for a solute that is uniformly applied to the soil surface in a pulse. The leaching surface is the surface that is obtained by plotting BTCs of many

different sampling locations alongside one another when the sampling locations are ranked according to the total amount of solute leached from them during the entire measurement period.

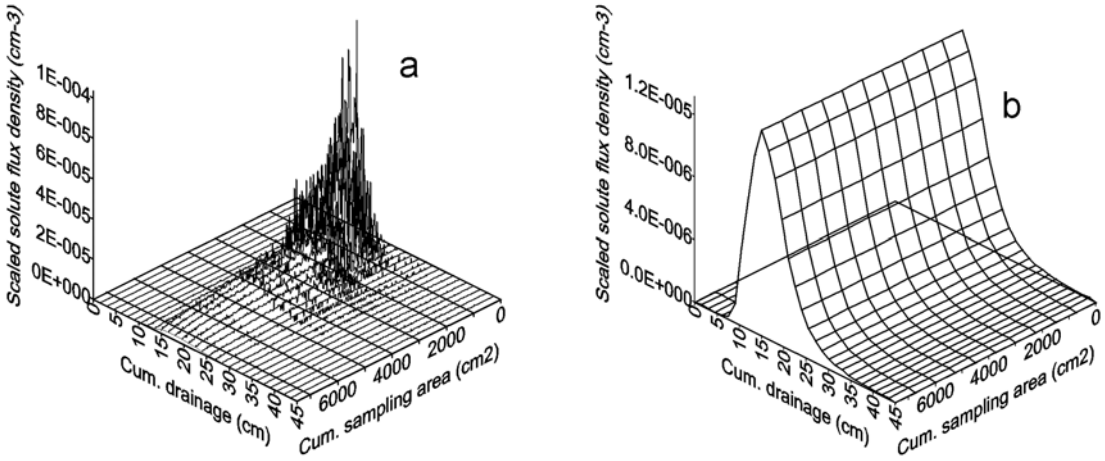

Figure 10. The leaching surface describing the spatio-temporal distribution of chloride leaching as observed under a large monolith lysimeter (a) (De Rooij 1996; De Rooij and Stagnitti 2002b). A strictly one-dimensional analysis eliminates the spatial variation and results in a very different leaching surface (b), based on the same data. Note the difference in the vertical scales.

Figure 10a shows the leaching surface as observed during a chloride-leaching experiment on a 1.00 m^2 surface area by 0.84 m undisturbed sandy soil monolith below which drainage was collected in 300 compartments of 5.0 × 5.0 cm area each (De Rooij 1996; De Rooij and Stagnitti 2002b). The leaching surface shows considerable concentration of leaching in a small portion of the total bottom area of the monolith, in addition to differences in solute arrival times between high-leaching and low-leaching regions. Reducing this spatio-temporal leaching pattern to a 1D simplification inevitably removes the spatial aspect of the leaching behavior. Figure 10b gives the resulting leaching surface, based on the same data. High- and low-leaching areas no longer exist, temporal differences between locations have been averaged out, and peak flux densities are underestimated by an order of magnitude. The loss of information resulting from the dimensional reduction is quite dramatic, but may nevertheless be acceptable if the spatial redistribution of solutes is judged to be of minor importance. On the other hand, the predicted leaching of toxic or reactive components may suffer from the incorrect representation of solute fluxes. Neither the SCM nor (at the moment) the FADE is able to model multidimensional leaching processes, and they can only produce degenerated leaching surfaces with loss of information such as that of Figure 10b.

SWOT analysis of the SCM, CDE, FADE and CTRW

For the analysis of the strengths, weaknesses, opportunities and threats (SWOT analysis) of the four modeling concepts, it is worthwhile noting that the SCM and the FADE, and to a lesser extent the CTRW, have been developed to correct well-documented shortcomings of the CDE. Their strengths are closely linked to specific properties of the CDE. We therefore first present the strengths and weaknesses of the CDE, and then those of the SCM, the FADE and CTRW. From these the main opportunities and threats of all four modeling concepts follow naturally, thus completing the SWOT analysis.

Table 3. Main strengths and weaknesses of the CDE equation

Strengths	Weaknesses
S1) The CDE has a proven record in applications for leaching of bulk solutes (e.g., salts).	W1) The tendency to normality of the solute distribution around the mean and its square-root evolution with time and travel distance are often too rigid to allow leaching predictions of small fractions of solutes (which is important when small amounts have large effects, as is the case with pesticides, phosphates, etc.), or to allow reliable calculations for large travel distances.
S2) As a consequence of S1, data sets and parameter values are available for many soils and climates.	W2) The assumption of Fickian transport has limited experimental or theoretical justification and appears to be wrong at scales between the decimeter and several meters. The dispersion coefficient serves as a lumped parameter representing all active solute-spreading processes in a given situation. The degree of lateral mixing determines how well the Fickian assumption of Brownian motion can serve as a proxy for the various spreading processes (Flühler, Durner and Flury 1996; Vanderborght et al. 2001). For many soils, the time and space scales of solute transport may be too small to justify the Fickian assumption (Sposito, Jury and Gupta 1986).
S3) The underlying concepts are easy to grasp.	
S4) The CDE is a linear second-order PDE, which is amenable to analytical and numerical analysis.	
S5) The CDE can be applied to multidirectional flow, arbitrary initial solute distributions and arbitrary solute applications.	
S6) The theoretical background, the underlying assumptions and the practical use of the CDE have been comprehensively developed and their advantages and disadvantages discussed in a vast body of literature.	W3) The lack of physical basis of the solute-spreading mechanism makes it difficult to upscale the CDE to field scale and larger scales. Parameter values at such scales must be considered effective. The limitations or Fickian transport referred to in W1 manifest themselves strongly in large-scale problems.
	W4) In most natural formations, long travel distances (in the order of 3 m or more) require the dispersion coefficient to increase with distance to relieve W1, introducing an additional, strictly empirical, parameter.

Table 4. Main strengths and weaknesses of the SCM concept

Strengths	Weaknesses
S1) The assumptions underlying the SCM are better justified physically than those of the CDE.	W1) The black-box nature of the travel time pdf requires calibration based on many measurements. Furthermore, the calibrated travel time parameters do not carry over to other conditions on the same location.
S2) The underlying assumptions are clear and explicit.	
S3) There is experimental support for the validity of the assumption of the stochastic nature of the travel time in some soils, even within plot-size areas; e.g., De Rooij and Stagnitti (2002b) show high levels of variation (inconsistent with efficient lateral mixing) between sampling locations with relatively rapid leaching, which carried the larger portion of the solute (Figure 10a), and Vanderborght et al. (2001) found evidence of stochastic-convective transport in several field and monolithic column experiments, especially in soils without horizontal features promoting lateral flow.	W2) Application to layered soils is possible but difficult (see discussion by Jury and Scotter (1994)); the travel time pdf transforms predictably with depth in non-layered soils only.
S4) The SCM makes solutes spread faster than the CDE does, which is especially important for field-scale solute transport (Butters and Jury 1989).	W3) The macroscopic flow must be nearly one-dimensional; complicated flow geometries require case-specific travel-time pdfs.
S5) The underlying concept is valid for any scale larger than the plot scale; when different soil strata, vegetation patterns etc. are included in the soil volume for which solute transport is calculated, the travel time pdf can be modified accordingly.	W4) The solute application must be uniform over the entire intake area of the soil volume of interest.

Table 5. Main strengths and weaknesses of the FADE model

Strengths	Weaknesses
S1) The physical and mathematical basis is well established in other fields of physics, and its use in soil physics is easily justified.	W1) The mathematical solutions are more complicated than those for CDE and the SCM.
S2) It has considerably more flexibility than both the CDE and the SCM, at the expense of one additional parameter. When the dispersion coefficient of the CDE is made dependent on travel distance, both the CDE and the FADE have two solute-spreading parameters.	W2) Very little is known about the relation between the parameter values and the nature of the solute transport process.
S3) The solute-spreading parameters are related to a physical transport process, and thus are likely to have more physical meaning than those of the CDE and the SCM.	W3) At the moment the FADE has only been applied to one-dimensional problems, and the extension to multidimensional problems, although possible, is mathematically complicated.
	W4) Representing particle migration by Lévy flights is not entirely correct, requiring an exaggeration of streaks of fast and slow flow in the main flow direction (Berkowitz et al. 2002).
	W5) There is still debate concerning the best method to estimate α and D_f (Zhou and Selim 2003).

Table 6. Main strengths and weaknesses of CTRW

Strengths	Weaknesses
S1) The CTRW generalizes solute transport processes; the stochastic and convective-dispersive flows being incorporated as limiting cases.	W1) Until recently, CTRW models have not been applied to unsaturated transport problems and hence have not yet been extensively evaluated in laboratory experiments (e.g. over different length scales) or in field trials.
S2) It can describe both Fickian and non-Fickian transport on a range of spatial and temporal scales.	W2) It requires a large volume of spatial and temporal measurements to determine transport parameters adequately.
S3) It has been demonstrated to describe anomalous transport in laboratory-scale applications (e.g. Berkowitz, Scher and Silliman 2000; Levy and Berkowitz 2003).	W3) It requires numerical iteration to determine solute parameters; several criteria may be used to judge goodness of fit, which may lead to different results.
S4) It can be used to fit BTC with long tails using just 2 fitting parameters	W4) Several aspects remain unknown: Is the dispersion parameter, β, invariant or does it change with, e.g., water content or increasing travel distance? Does CTRW tend to Fickian flow over large travel distances?

Opportunities and threats to the CDE

Given the above, the CDE is most reliable when used to model movement of bulk solutes over distances of a few meters or less in moderately sized soil volumes. On smaller scales, mixing is insufficient to validate the Fickian assumption, and on larger scales large heterogeneities enhance solute spreading. The CDE is likely to perform well when describing transport of salts and nutrients through laboratory columns, lysimeters or instrumented field plots, and possibly through drained fields, where dispersion creates a limited amount of solute spreading in comparison with the travel-time variation caused by the geometry of the flow lines to drains and/or ditches.

The CDE is likely to lose terrain to the SCM and the FADE when intricate details of leaching behavior need to be simulated (e.g., pesticide transport), when large travel distances are involved (unsaturated-saturated flow; deep unsaturated zones). Also, modeling solute transport in large soil volumes (regional scale) that invalidate the Fickian assumption remains difficult with the CDE.

Opportunities and threats to the SCM

The SCM can in principle outperform the CDE for the limited subset of problems for which the SCM is well suited. It is simpler to implement than the CDE and often better reproduces observed BTCs. However, the flow must be essentially 1D and the solute application needs to be uniform. This makes the SCM well posed to model transport of uniformly applied solutes (e.g., fertilizers, Jury and Scotter 1994). Flow to tile drains etc. requires a modified travel-time pdf. Jury (1975) derived an analytical travel-time distribution for saturated flow towards tile drains. If such an approach is taken, the stochastic element of the SCM is removed. In principle, one could implement any desired spreading mechanism to work out solute spreading in the resulting analytical description of the flow system. The SCM seems to be particularly appropriate for modeling regional-scale transport of contaminants from diffuse sources between the soil surface and the phreatic aquifer.

The limited range of application of the SCM leaves open the possibility that more general numerical codes based on the CDE will continue to be used for problems for which the SCM would have been more appropriate. In the more distant future, the more general FADE can compete with the SCM at scales unsuitable for the CDE, especially if the generalization to multi-dimensional systems proves successful.

Opportunities and threats to the FADE

The FADE is very new and has considerable potential: it is more flexible than the CDE and the SCM, and should be applicable to any problem that can be tackled by either. Its computational complexity will probably not strongly hamper its application. Its similarity to the CDE should facilitate the incorporation of the FADE in codes that first solve Richards' equation, then the solute transport equation. Similarly, the inclusion of sorption, chemical reactions, interactions with crops, etc. should be relatively straightforward since none of these processes are directly connected to the terms containing fractional derivatives.

The fact that the FADE produces non-Brownian motion on any scale of application makes it a very suitable candidate for quantifying solute transport problems that cover a wide range of scales (e.g., a combined soil-aquifer system). However, both the CDE and the FADE are special cases of a continuous-time random-walk (CTRW) model, where the CDE in particular represents highly restrictive conditions. Berkowitz et al. (2002) pointed out that the FADE requires streaks of high and low conductivity in the flow domain that are usually not observed in natural porous media. These elongated streaks offer solute particles a wide range of lengths of pathways with different velocities from which non-Fickian solute spreading can emerge. Also, Lévy flights of solute particles lead to a diverging second moment of the solute plume, which is unlikely to happen in real-world plumes (Berkowitz et al. 2002). Hence, although the physics of the FADE is more realistic than that of the CDE, CTRW models may still prove superior in the future.

A considerable threat to widespread application of the FADE is the complexity of the multidirectional fractional derivatives. If no easy way can be found to implement these numerically, many of the limitations that plague the SCM will affect the applicability of the FADE.

Opportunities and threats to CTRW

CTRW models potentially offer significant benefits to solute transport modeling, particularly in regard to describing processes which may neither be stochastic-convective nor convective-dispersive but some approximation of these. The model

algorithms are not necessarily easy to apply but they are no more difficult than other parameter-fitting models. Many more field and laboratory studies are required to validate fully the suitability of this approach to solute transport studies. In particular, assumptions concerning the dispersion parameter, β, (e.g., spatial or temporal invariance) will require checking on a wide variety of soil types (e.g. aggregated vs. fractured vs. sandy media) and different solute application methods (e.g. continuous, pulse, irregular etc.). The relationship between FADE and CTWR also needs to be further clarified.

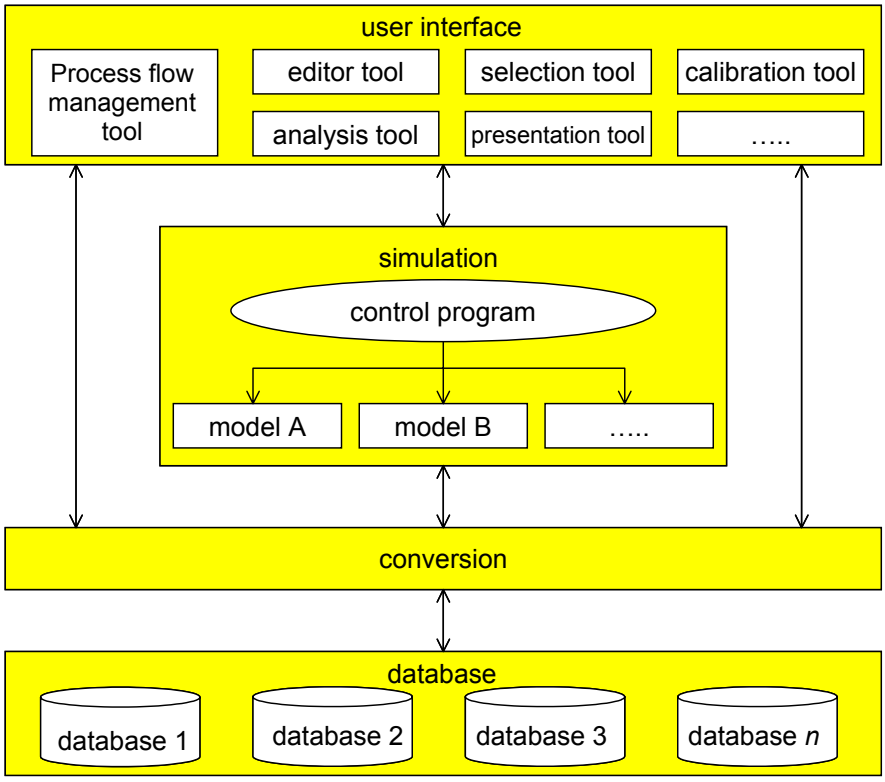

Figure 11. General architecture of framework for model coupling (Blind, Van Adrichem and Groenendijk 2001a)

Model integration versus model coupling

The increasing computational power tempts to analyse problems of ever-increasing complexity. Therefore interest in multi-dimensional problems is growing. Scientists also want to combine more processes, including their interactions (Greiner 2003). For example, plant growth models are combined with soil process models. The question then arises is how to combine these models. When processes are independent or interact only in one direction, models can be run apart from each other. For instance soil water flow affects pesticide transport, but pesticide transport does not affect soil water flow. However, many processes have interaction in both directions. For such cases two approaches can be followed: model integration or model coupling.

Model integration means source-code integration. In this way it is possible to combine the processes at the smallest time scale. Flow of information between the constituent models occurs in the correct order at the correct times. This is of particular interest when all processes have the same order of characteristic system times. A good example of this approach is the integration of solute transport and water movement in

porous media. A major drawback is that integrated source codes become so complex that maintenance is difficult, and only large organizations with specialized research groups are able to improve the code.

In case of model coupling, the main core of the models is left unchanged. Alterations are needed only at a higher level to allow for communication between the models. Model coupling requires a coupling shell or framework. This is a piece of software that calls underlying models, takes care of the interaction between the underlying models, and handles input and output of the models (Figure 11). Development of such a framework requires analysis of the proper subdomains, type of models, information flow between the models, and kind of databases. An example of a hydrological domain analysis is given in Figure 12 (see Color pages elsewhere in this book). These domains were considered as natural building blocks of the hydrological system, with each domain having its specific processes and communication requirements (Van der Wal and Van Elswijk 2000).

At present, hydrological frameworks are not so sophisticated that models can be simply added by researchers (the so-called 'plug-and-play' principle). Also, the linking of models through a coupling shell or framework and maintaining such systems is usually very time consuming and budget demanding. An example of a hydrologic framework can be found in Blind, Van Adrichem and Groenendijk (2001a; 2001b). Maybe, the simplest coupling shell is one that primarily takes care of the synchronization of the underlying models and that provides a protocol for data exchange between the models. The FSE4 shell (Rappoldt and van Kraalingen in prep.) is an example of such a synchronization shell. Under FSE4 the original models stay intact. Each model needs an interface that can handle standard calls from FSE4 and translate these to calls to the underlying model. Furthermore, data exchange between models occurs at the level of the interface. Once the shell and communication manager are fully developed, it does not need further maintenance. Coupling can then be achieved by the modelers themselves by maintaining the interfaces and their own models.

A brief SWOT analysis of model integration and model coupling is provided in Table 7.

Examples of model coupling

The Australian framework APSIM (Agricultural Production Systems Simulator) was developed to simulate biophysical processes in farming systems with special attention to economic and ecological effects (Keating et al. 2003). APSIM consists of several biophysical modules (e.g., crop growth, soil water movement, soil N and P dynamics), a set of modules to characterize a management scenario, various modules that handle input and output, and a simulation engine that drives the processes.

The coupled model 'Waterpas' (De Vos in prep.) consists of the sub-models SWAP for soil water movement, CNGRAS (Conijn in prep.) for grass growth, and a grassland usage planner at the farm scale. 'Waterpas' calculates the effects of regional water management on farm management and economic yields. For environmental purposes a soil nitrogen transport model will be included as well.

Coupling of the 2D soil model FUSSIM2 (water flow, solute transport, root uptake; (Heinen 1997; 2001; Heinen and De Willigen 1998; 2001) with CNGRAS (Conijn in prep.) is an example in which several instances of a single source code (CNGRAS) are used. This requires complete storage of the status of each instance by the model.

Table 7. SWOT of model integration and model coupling

	Model integration	Model coupling
Strength	▪ processes can be combined at the smallest time scale ▪ information flow between the several components occurs in the correct order at the correct times	▪ original models stay intact ▪ models can be developed and maintained independently ▪ depending on the required accuracy different model types can be chosen
Weakness	▪ source codes become very large and sometimes complex, so that maintenance becomes difficult ▪ small research groups are responsible for integrated models that cover a wide range of disciplines	▪ interaction with a framework or shell requires overhead in computation time ▪ the setup and maintenance of a proper model framework requires substantial financial investments and a proper organization
Opportunity	▪ identify and quantify feedback relationships between processes that cannot be found experimentally	▪ identify and quantify feedback relationships between processes that cannot be found experimentally ▪ in principal, model coupling can reach the plug-and-play status at some time in the future
Threat	▪ integrated models become so complicated that only a few research institutes can afford to develop and maintain such models	▪ increasing combination of models with different time and spatial scales may cause overkill in computation times

Such a combination allows analysis of differences in management at a 2D cultivated field. For example, Assinck, De Willigen and Van Beek (2002) investigated the effect of no fertilization in the strip along a drainage canal on nitrogen leaching. Nitrate leaching was effectively reduced due to nitrogen uptake by grass and due to denitrification in the non-fertilized strip. With the same coupled model, Conijn and Henstra (2003) studied the effects of fertilizer strategies on yield and nitrogen losses in case of mown grassland. From the strategies considered in their study they concluded that fertilizer application tuned with mineral-N content in the top soil (0-30 cm) resulted in reduced nitrate leaching with minimal yield decrease.

Another type of coupling is the linkage between process models and geographic information systems. Examples are DSSAT (Decision Support System for Agrotechnology Transfer) (Jones et al. 1998) and the combination SWAP-ArcView (Kroes et al. 2002).

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