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A random-walk approach for simulating wastewater transport and transformations in the unsaturated zone

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Abstract Point sources of wastewater in the subsurface are a potential threat to groundwater quality. Modelling wastewater transport and transformation requires dealing with a complex system of processes and interactions between solutes as well as between the solutes and the solid phase. Therefore the process-based reactive transport model WSTM (Water and Solute Transport Model) was developed, based on the random walk approach and fulfilling the Fokker-Planck equation for the unsaturated water flow. The main focus of this paper is on the mathematical formulation and applications of the model.

Keywords random walk approach; reactive transport modelling; unsaturated zone

INTRODUCTION

Studies on groundwater and soil contamination require quantitative analysis of the migration of reactive substances. Predicting the effect of wastewater exfiltration from damaged sewers on groundwater quality makes especially necessary the understanding of the complex system of processes and interactions between solutes, as well as between the solutes and the soil matrix within the unsaturated zone.

Mathematical models for simulating this phenomenon consist of a set of coupled partial differential equations that describe the mass conservation of each species (Bear, 1979). In general, these partial differential equations are solved by finite difference method or finite element method. As they are based on time and space discretizations, the size of the time and space steps should be chosen wisely; otherwise the numerical solutions may be inaccurate or unstable (Sun, 1996). Moreover, they suffer from numerical dispersion and high computational effort. To avoid numerical dispersion, various Langrangian and Eulerian-Lagrangian algorithms have been developed (e.g. Celia *et al*., 1989), such as the random walk method (Prickett *et al.*, 1981).

This paper illustrates further development of the numerical method presented by Bücker-Gittel *et al.* (2002). This method is based on the random walk approach, balancing the water and associated mass transport in the unsaturated zone. It allows the quantification of the mass transfer between different phases (i.e. the mobile fluid phase, and immobile solid phase) and of the reactive processes. It is applied for investigating the plume development from a point source (e.g. sewer leak) in the unsaturated zone and its impact on groundwater. One advantage of the model is that the water and the solute transport are calculated simultaneously, without having to first run a flow model and then a transport model, saving simulation effort.

MODELLING APPROACH

Water transport in the unsaturated zone

Transport of dissolved solutes in the unsaturated soil zone depends on the unsaturated water flow, which is usually described by the Richards' equation:

$$\frac{\partial \theta}{\partial t} = \vec{\nabla} \cdot \left[K(\theta) \left(\vec{\nabla} \psi(\theta) + \vec{e_z} \right) \right] \tag{1}$$

where $\vec{e_z}$ is the unity vector in the vertical direction. This equation relates the temporal change in the volumetric water content $\partial\theta/\partial t$ ($cm^3\ cm^{-3}\ s^{-1}$) to the gradient on the water suction $\nabla\psi(\theta)$ and to the hydraulic conductivity $K(\theta)$ ($cm\ s^{-1}$). The variability in the volumetric water content θ ($cm^3\ cm^{-3}$) is limited by the maximum value of the saturated water content θ_s ($cm^3\ cm^{-3}$) (theoretically the porosity) and by the residual water content θ_r ($cm^3\ cm^{-3}$).

With regard to the microscale variability of the pore sizes and the associated capillary forces, equation (1) could be formulated as a Fokker-Planck equation for the volumetric water content θ (Bücker-Gittel *et al.*, 2002):

$$\frac{\partial \theta}{\partial t} = \underbrace{\vec{\nabla} \cdot \left(D \vec{\nabla} \theta \right)}_{(A)} + \underbrace{\frac{\partial}{\partial z} \left(\left(\frac{K(\theta)}{\theta} \right) \theta \right)}_{(B)} \tag{2}$$

with the capillary diffusivity $D(\theta)$ ($cm^2\ s^{-1}$) defined as:

$$D(\theta) = -K(\theta) \frac{d\psi}{d\theta} \tag{3}$$

Equation (2) balances the water transport in the unsaturated zone. The diffusive term (*A*) accounts for the spreading of the seepage water due to capillary forces. Term (*B*) describes the vertical movement due to gravity (i.e. advection).

Solute transport in the unsaturated zone

Solute transport, including the reactions and the mass transfer between the phases in the unsaturated zone, is treated similarly to the transport in the saturated zone. It is associated with the water flow, which is determined by advection (gravitational force) and by the capillary diffusivity (capillary force). In contrast to the saturated zone, in the unsaturated zone the capillary diffusivity is dominating dispersion and molecular diffusion. Hence, the solute mass transport equation for the concentration C ($mg\ L^{-1}$) is given by:

$$\frac{\partial \theta\, C}{\partial t} = \vec{\nabla} \cdot \left(D \vec{\nabla} \theta\, C \right) + \frac{\partial}{\partial z} \left(\left(\frac{K(\theta)}{\theta} \right) \theta\, C \right) \tag{4}$$

Random walk approach

In general, the random walk approach considers the mean transport velocities as well as random velocities fluctuations within a REV (representative elementary volume) of the porous media. Here, the capillary forces on the pore scale generate these fluctuations.

As the Richards' equation is reformulated as a Fokker-Planck equation (2) for the water transport, the random walk approach can be used for balancing the water flow in the unsaturated zone by moving particles representing a defined water volume V_w. Furthermore, the similarity between equations (4) and (2) leads to the representation of the mass transport by defining mass loadings for each particle, m_p^k (k being the solute index). The total displacement of a randomly moving particle p consists of an advective and a dispersive movement and is calculated by (Bücker-Gittel *et al.*, 2002):

$$\Delta x = \frac{\partial D}{\partial x}\Delta t + Z\sqrt{2D\Delta t} \tag{5}$$

$$\Delta y = \frac{\partial D}{\partial y}\Delta t + Z\sqrt{2D\Delta t} \tag{6}$$

$$\Delta z = \left(\frac{\partial D}{\partial z} - \frac{K(\theta)}{\theta}\right)\Delta t + Z\sqrt{2D\Delta t} \tag{7}$$

where Z is a normally distributed random variable with zero mean and unit variance. To account for the non-uniform flow field, the advective step includes a correction term $\partial D/\partial z$. The physical meaning of this term is the conservation of particle flux due to dispersion between two locations with different assigned flow velocities (Hoteit *et al*., 2002).

To balance the water content and the solute masses, the model domain is divided into uniform cells of constant length, $\delta x = \delta y = \delta z$. The number of particles defines the volumetric water content θ. The dissolved concentration C_d^k (i) is determined by summing up the mass loadings for each solute:

$$C_d^{\,k}(i) = \frac{\sum_{p=1}^{N_p} m_p^{\,k}}{\theta\, dV} \tag{8}$$

where N_p is the number of particles per cell, dV is the cell volume (cm^3), i denotes the cell index and k is the solute index. Furthermore, the hydraulic conductivity $K(\theta)$ and the capillary diffusivity $D(\theta)$ are calculated for each cell by using the Brooks & Corey (1966) relationship.

By adding particles an infiltration source is simulated. These particles are moved, reflected at the closed boundaries and removed when crossing an open boundary (e.g. groundwater table, free outflow).

Mass exchange

When a particle p moves, it represents the mobile fluid phase and brings the solute mass from one location to another one. At the same time it exchanges mass with the

immobile solid phase (i.e. the cell). In WSTM this exchange takes place between individual particles and the respective cell. For example, in the case of linear sorption under equilibrium conditions, there are two masses to be dealt with within a cell at any time: the dissolved mass $m_d{}^k$ (mg), and the sorbed mass $m_s{}^k$ (mg):

$$m_d{}^k(i) = \sum_{p=1}^{Np} m_p^k \tag{9}$$

$$m_s{}^k(i) = f^k(i)\, m_d{}^k(i) \tag{10}$$

The exchange coefficient $f^k(i)$ is given by:

$$f^k(i) = K_d \rho_s \frac{1-n}{\theta} \tag{11}$$

where ρ_s (g cm^{-3}) is the solid density, n (–) is the porosity of the domain and K_d (L kg^{-1}) is the distribution coefficient. At each time step the particle mass has to be updated with respect to that mass exchange. Thus the mass carried by the particle, or the concentration in a cell, is continuously changed as a particle passes through a cell and exchanges masses with it. The sorbed/desorbed mass at every given location in time and space is known by the exchange coefficient $f^k(i)$ and the dissolved mass.

NUMERICAL INVESTIGATIONS

A three-dimensional numerical example is considered for the investigation of the effect of linear sorption on the solute transport in an unsaturated homogeneous soil. The dimensions of the model domain were 0.6 × 0.6 × 1.5 m (Fig. 1) and it was divided into uniform cells of length δx = 0.05 m. The lateral boundaries as well as the top boundary were defined as no-flow boundaries and the bottom boundary was represented by saturated conditions (i.e. groundwater table at z = 0 with $\Psi = 0$). At the elevation z = 0.95 m, particles were injected characterizing a sewer leak. The initial volumetric water content distribution was calculated for hydrostatic conditions.

From t = 0 to t = 3600 s, water mixed with a conservative solute and a sorptive solute was infiltrated with an infiltration rate Q = 0.0216 m^3 day^{-1} into an initially clean environment (C_0 = 0). The concentrations of both solutes were assumed to be 1 mg L^{-1}. After t = 3600 s, the injected water became clean. The model input data are given in Table 1, where α_{vG} and n_{vG} are the van Genuchten parameters (van Genuchten, 1980). Figure 1 illustrates the development of the plume for the volumetric water content (Fig. 1(a)), and for the solutes (Fig. 1(b) and (c)). For comparison reasons only, the dissolved part of both solutes is presented here.

At the beginning of the infiltration the wetting front was almost radial, while with increasing time the water distribution showed more a downward than lateral spreading behaviour (Fig. 1(a)). Only the soil near the leak was saturated, whereas the parts down to the groundwater table remained unsaturated. Due to this saturation the area above the sewer leak behaves similar to a “capillary fringe” resulting in a large increase in the volumetric water content.

The distribution of the conservative solute that was not adsorbing on the soil matrix but remained in the fluid phase shows a high dilution effect (Fig. 1(b)), with the

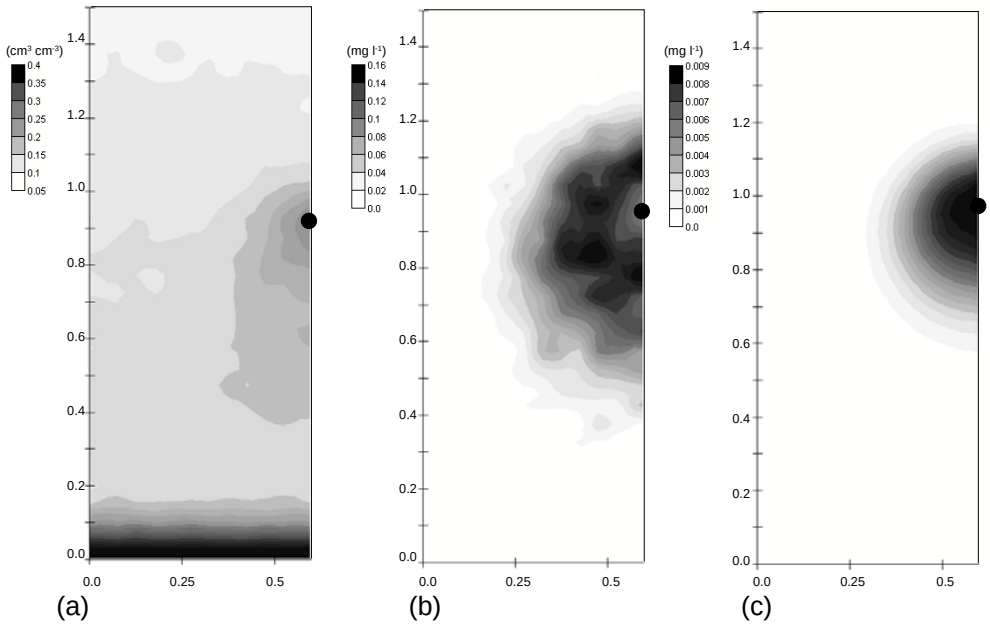

Fig. 1 Distributions of: (a) volumetric water content, (b) concentration of conservative solute, and (c) concentration of sorptive solute, at t = 5400 s.

Table 1 Model input data.

Solute	K_{sat} (m s^{-1})	θ_s (cm^3 cm^{-3})	θ_r (cm^3 cm^{-3})	α_{vG} (m^{-1})	n_{vG} (–)	ρ_s (g cm^{-3})	K_d (L kg^{-1})
A	1×10^{-4}	0.4	0.06	6.0	1.7	2.65	0
B	1×10^{-4}	0.4	0.06	6.0	1.7	2.65	5.8

concentration about 10 times lower than the input concentration. The plume of the reactive solute (Fig. 1(c)) has been significantly decreased in comparison with the conservative one (Fig. 1(b)) because a part of the solute mass, which was first diluted in the fluid phase, was then adsorbed onto the soil matrix.

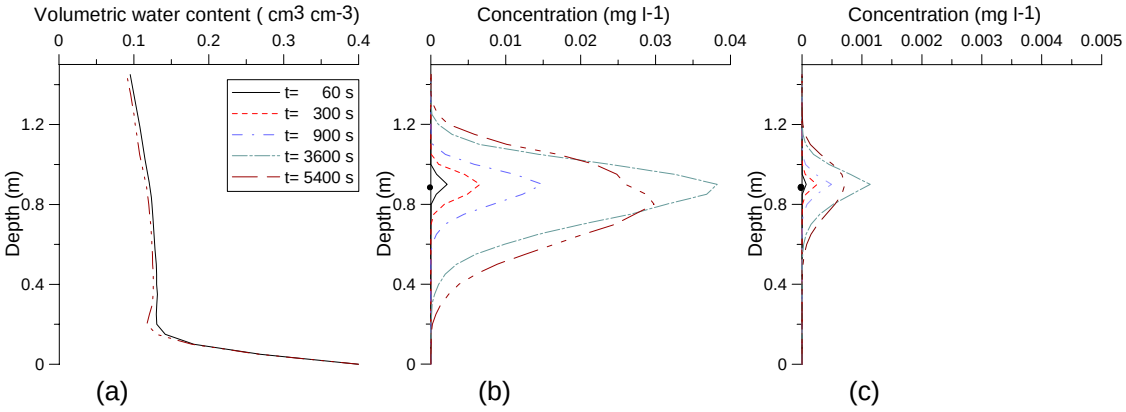

Fig. 2 Evolution of: (a) volumetric water content, (b) concentration of conservative solute, and (c) concentration of sorptive solute.

Figure 2 shows the layer-wise averages of the water content and solute concentrations for different simulation periods. The average volumetric water content (Fig. 2 (a)) was relatively constant over the plotted time periods. The conservative solute reached an average concentration of 0.04 mg L^{-1} after 1 hour of infiltration. After this time, the solute concentration decreased gradually and was flushed out with the incoming clean water. Plotting the sorptive solute for the same periods, the strong uptake of the solute by the matrix, together with the dilution effect, reduces the maximum concentrations in the dissolved phase by 95%. Therefore, a significant part of the solute was stored in the soil for a relatively long time, causing a potential risk for the groundwater resources. The solutes reaching the groundwater were highly diluted and retarded.

CONCLUSIONS

If the Richards' equation is reformulated as a Fokker-Planck equation for the water transport, the random walk approach can be used for balancing the water flow in the unsaturated zone by moving particles representing a defined water volume. Also, the mass transport can be represented by defining mass loadings for each particle. Thus, the unsaturated water transport and mass transport can be computed together. This approach is implemented in the numerical model (WSTM). It was applied to simulate a sewer leak infiltration in unsaturated soils considering conservative and sorptive solutes. The distributions of the water content and the solutes concentration are well represented.

For the complete assessment of wastewater impacts on soils and groundwater, detailed understanding of migration and transformation of substances in the subsurface is required. The implementation of the relevant transformation processes (e.g. redox-reactions) into the numerical model enables detailed investigation of their interactions on transport. Simulation results considering transformation processes will be validated by the use of the experimental results in order to provide a tool with predictive capability.

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