SIMULATION IN VADOSE SOIL ENVIRONMENT

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ABSTRACT

Emphasise will be given to simulation concepts for the vadose zone and to the limitations of available software, e.g. related to boundary conditions. Classical water and solute transport formulas are investigated in relation to the used software. A practical approach is chosen to support the theoretical considerations, hence three simulation applications in very different fields: a) quantity measurement of soil water movement, b) thin layer in the vicinity of a foundation and c) solute transport simulation of a column experiment are summarised. The selected examples should especially enable engineers working in the field of water and environment an easier approach to simulation task and the underlying theory. A clear distinction is also made between skills and knowledge.

INTRODUCTION

Simulation tools are still object to an increase of importance. However running a computer program (skill) is not sufficient for a simulation. For the interpretation of simulation results related to environmental issues or to react adequately to arising obstacles in an application a good physical understanding and at least some mathematical background (knowledge) is indispensable. This fact is often not seen very clearly, hence the discrepancies between users and developers are increasing. One attempt as seen by the authors is to demonstrate simulation concepts and methodologies in a context of applications. A link to measurements will be provided, on one side to obtain necessary input data and on the other side to check the plausibility of physical experiments. A further advantage of simulation is that by varying parameters the heterogeneities of the natural environment can be taken into account.

SIMULATION CONCEPTS

A good simulation of water movement is one of the necessities for all simulations in the vadose zone. The basic flow equations are not treated, because they can be found in many text books (e.g. Bear and Verruijt 1990) and should be in any case part of a good hand book. Therefore only an overview of the respective components of solute transport, like adsorption, retardation and kinetic terms and the presentation in respective equations is given in the following.

Chemical nonequilibrium (NE) model

A two-site chemical (NE) model where the adsorption term consists of two components, one governed by equilibrium (Eq)-adsorption and the other by first order kinetics, has been proposed by Selim et al. (1976) and Cameron and Klute (1977). The sorption or exchange sites in this model are assumed to account for instantaneous adsorption (type-1 sites) and time dependent kinetic adsorption (type-2 sites).

$$(1+\frac{f\rho K_d}{\theta})\frac{\partial c}{\partial t}+\frac{\rho}{\theta}\frac{\partial s_2}{\partial t}=D\frac{\partial^2 c}{\partial x^2}-v\frac{\partial c}{\partial x}$$

$$\frac{\partial s_2}{\partial t}=\alpha\big[(1-f)K_d c-s_2)\big]$$

where f = fraction of all sites occupied by type-1 sorption sites, ρ = bulk density, θ = water content, K_d = distribution coefficient for linear adsorption, c = solute concentration, t = time, D = effective diffusion-dispersion coefficient, v = pore water velocity, s_2 = solution concentration (type-2 sites) and α = first order rate coefficient.

Physical NE model

The liquid phase is divided into a mobile and immobile region within the two-region model. The one-dimensional solute transport for an exchanging solute during steady state flow through a homogeneous porous medium includes an Eq- adsorption-desorption process (van Genuchten & Wierenga 1976). The model can be described as following

$$(\theta_m+\rho f K_d)\frac{\partial c_m}{\partial t}+[\theta_{im}+(1-f)\rho K_d]\frac{\partial c_{im}}{\partial t}=$$

$$=\theta_m D_m\frac{\partial^2 c_m}{\partial x^2}-\theta_m v_m\frac{\partial c_m}{\partial x}$$

$$[\theta_{im}+(1-f)\rho K_d]\frac{\partial c_{im}}{\partial t}=\alpha(c_m-c_{im})$$

where c_m, c_{im} = solute concentrations in the mobile, immobile liquid phases, with corresponding volumetric water contents θ_m and θ_{im} respectively, D_m = apparent diffusion coefficient of mobile liquid phase, v_m = average mobile pore water velocity, α = first order mass transfer

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coefficient and f = mass fraction of solid phase in direct contact with the mobile liquid phase.

SIMULATION APPLICATIONS

Miniature Lysimeter

It is commonly agreed that water movement in the soil is not accessible to direct observations (Flühler und Roth 1999), nevertheless devices, so called miniature lysimeters, are proposed for direct observation. In an experimental field three miniature lysimeters (or soil water sampler) and equipment for measurement of soil water content and tension were installed. To achieve controlled boundary conditions the soil was saturated and then covered with a plastic foil to prevent evapotranspiration. The change of water content and tension was recorded with a data logging device. The outflow of the lysimeters was collected in sampling bottles by means of a pressure plate in combination with a vacuum pump. Two lysimeters (SWS2, SWS3) were operated with constant negative pressure heads and one lysimeter (UMS1) was automatically adjusted to the soil water tension of the surrounding soil. SWS3 was hydrologically separated. The change of water content was evaluated with the instantaneous profile method. The amounts of water collected with the lysimeters varied substantially and did not match with the storage change and the applied amount of water (Table 1).

Table 1: Results of Field Experiment

Water collected in lysimeters 17.9.98-19.9.98	
Device	applied tension
UMS1 11.1 mm SWS2 5.7 mm SWS3 27.4 mm	variable, adjusted to surrounding soil tension 200 hPa constant 200 hPa constant, hydrological separated
Calculated change of water content = 28 mm (Max. storage	
Applied amount approx. 30 mm	

To demonstrate the water collecting ability and to show the flow pattern in the vicinity of a miniature lysimeter a simulation of deep percolating water is performed. The simulation allows a physical reasoning of the system behaviour and insight into the flow process, hence the discrepancies of water flow rates are explainable.

For this task the software SEEP/W (1991) for finite element seepage analysis (GEO-SLOPE International Ltd.) was used. Besides other features this software allows saturated and unsaturated flow calculations in two dimensions. The presented axialsymmetric problem was simulated for transient flow and constant boundary conditions. Initial conditions were obtained from a steady state run by calibration to field measurements. Irrigation according to field experiment was 30 mm for 60 minutes. Main input parameters are:

- number of soil profile layers,
- soil water retention curve and
- soil water content - hydraulic conductivity relation.

Simulation results

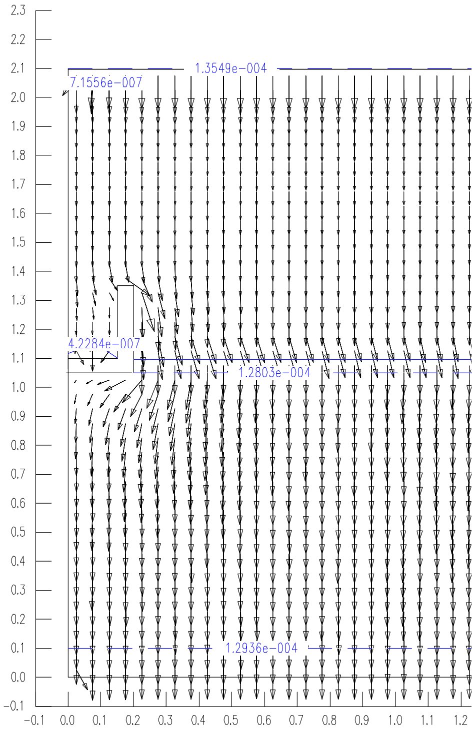
The conditions of SW2 are used for demonstration. Cumulative flow rates at different time steps are calculated (Table 2). For the calculation of flow rates cross-sections are specified within the domain. For this example the columns in Table 2 present cross-section values.

Table 2: Cumulative In and Outflow of the Simulation Domain

t [min]	SW2	Drainage	Irrigation
5,0	1,87	17,47	2,64
30,5	3.36	17,47	17,64
79,7	6,59	38,50	30,43
158,9	10,75	46,12	30,50
491,7	14,20	55,04	30,50
1358,1	17,94	71,73	30,65
3894,5	22,12	98,82	31,00

The irrigation (inflow) increases slightly which is not in accordance with the boundary condition (applied water), because the flow through this cross-sections also includes the drained water of the first layer. The soil profile was near saturation at the beginning, therefore the outflow is increasing until a steady state condition is reached. The line in Table 2 indicates when the maximum of water storage change was measured. To give a physical reasoning of this result the flow pattern with time is presented in Figure 1.

a) for time step 1



b) for time step 10

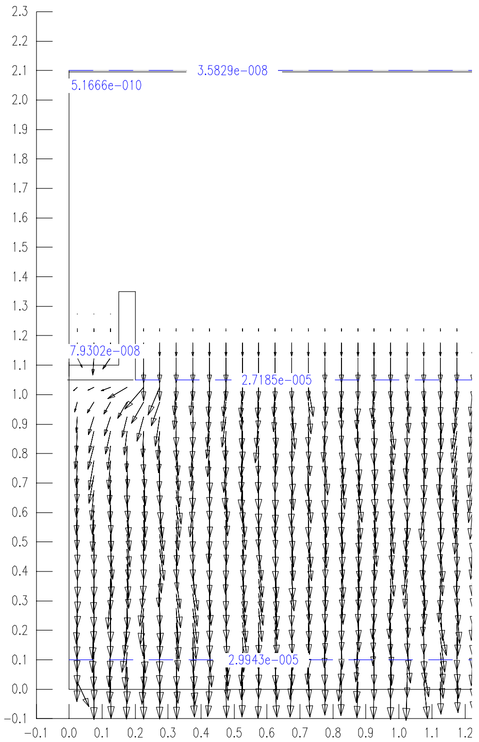


Figure 1: Flow Pattern in Soil Body Containing a Miniature Lysimeter a) for time step 1, beginning of irrigation; b) for time step 10 (1,33 hours), drainage of soil profile

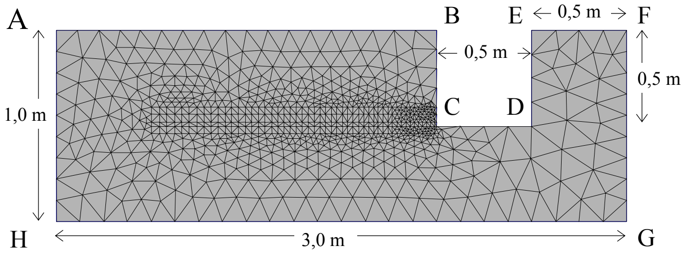
From the flow vector presentation it is clearly seen that the water movement is attracted to pass the lysimeter instead of entering it. Also the movement of the drainage front is visible.

Foundation

The geotechnical background of this investigation is to evaluate the influence of a geotextile on the moisture content to reduce swelling and shrinking. The placement of a permeable geotextile should enable the control of the water content in the vicinity of a foundation.

The computational concerns are how do treat a thin layer as an internal boundary and the discontinuity of the permeability with space as well as in time.

Computations were performed using the 2-dimensional Finite Element model HYDRUS_2D (Simunek et al. 1999). This software is selected because it allows atmospheric boundary conditions as compared to the previous used SEEP/W. The mesh and geometry are represented in Figure 2.



AH and FG : impermeable
BCDE : impermeable (boundary of the foundation),
AB : atmospheric boundary condition
HG : boundary of a drainage layer (free drainage at bottom) or ground water table.

Figure 2: Finite element mesh and geometry

Soil properties were utilized by using van Genuchten´s equation.

The first concern is related to the mesh generation. The used software does not allow to choose a regular (triangular) mesh, but with auxiliary lines at least in the vicinity of the thin layer a regular net was forced to develop to improve the stability of the computation. Stability considerations are also a matter of the abrupt changes of permeability. The refinement of the mesh has to be in relation to the thickness of the geotextile. For the calculation (steady state computation) of initial conditions the thin layer was considered first as impermeable in the following transient simulations. Because it is not possible to apply straight forward varying permeabilities with time, the transient computation had to be done in two steps. First it was continued with the impermeable layer until a desired water pressure head above the geotextile was reached (Figure 3). The simulation is then stopped, the water content and water tension is stored to be used as initial condition for the following second phase with changed input data. The key feature is the change of the permeability of the control layer. If the pressure head above the thin layer becomes lower than a selected threshold value the computation has to be stopped again and the process may be repeated starting with step one and so on.

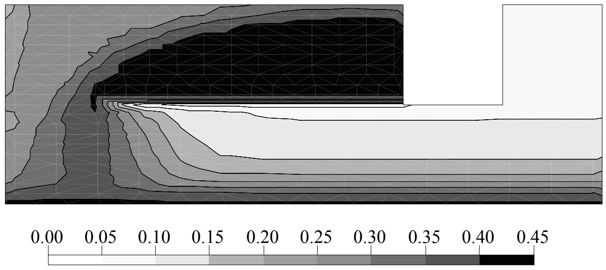


Figure 3: Water Content Simulation of Step One after 17 Days

The dark parts (0,45) in the graph indicate a saturated soil. Following this stepwise procedure the evaluation of controlling the water content could be performed satisfactory.

Solute transport

The software HYDRUS_2D is capable to calculate solute transport as well and includes equations for two-site and mobile/immobile models. A stationary column experiment performed by Shukla (1998) with different pore water velocities (v_p) and competing chemicals $Ca^{2+}Br_2^-$ and $Mg^{2+}Cl_2^-$ was simulated. Parameters used as input for the numerical models were obtained by inverse modeling with the program CXTFIT (Toride et al. 1995). In Figure 4 the sum of residua is shown for one case where $v_p = 0.5$ cm/h, the experiments and other simulations have been described in more detail by Fellner (1999) and Klepsch et al. (2000).

HYDRUS_2D	*Eq*	*two-site NE*	*two-region NE*
$\sum(\mathbf{C}_{\mathbf{gem.}} - \mathbf{C}_{\mathbf{sim.}})^2$	0.044	0.033	0.034

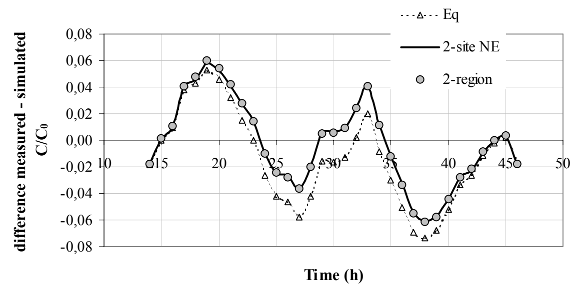


Figure 4: Difference Measured – Simulated Breakthrough Curve (BTC) Applying Eq model, Two-Site NE-Sorption and Mobile/Immobile Concept ($v_p = 0.5$ cm/h, $K_d = 0.186$ dm³/kg, f = 0.113, α = 2e-3 h; and $\theta_{im} = 0.150$, f = 0.657, α = 5.2e-4 h^{-})

Although no calibration was performed a quite good correlation between simulated and measured BTCs was found, with slightly better results for the NE models as compared to the Eq-model (the „classical“ convection-dispersion equation). Nevertheless it shall be emphasized that the model parameters better should be determined independently to be able to use the models in a predictive way. One also has to be aware that – generally - the simulation results may not be over-interpreted. For instance, in reality both sorption and physical NE phenomena are complicated and often coupled processes. The models' limits have to be known, but also the situations where an easier Eq concept could be used instead of the more complicated NE equations which result in more unknown parameters, numerical difficulties etc.

Other complications the user of a simulation tool has to be conscious of are: no sufficient input-data are available, a lack of exact (and not too expensive) methods for measurement of unsaturated hydraulic properties, spatial and time dependent variability of soil properties and transport parameters, superposition of hydraulic and solute transport parameters measured in laboratory to higher scales, or the risk of non-unique solutions.

HYDRUS_2D proved to be very useful, however a need for additional features occurred for certain applications. The original FORTRAN 77 source code of HYDRUS_2D, which the authors of the software had made available, was slightly modified to run as a stand-alone DOS model without the user interface. As compiler Fortran Powerstation (Version 1) was used. With this modified version input files can still be created via the graphical user interface and output files can be viewed by it. Thus, some additional subroutines that may be useful in specific cases can be incorporated into the program and probable lacks of a software at least are a little compensated (Figure 5). These extensions require additional input data, realized by a separate input-file ("add.in") and supplementary variables in the original file "selector.in".

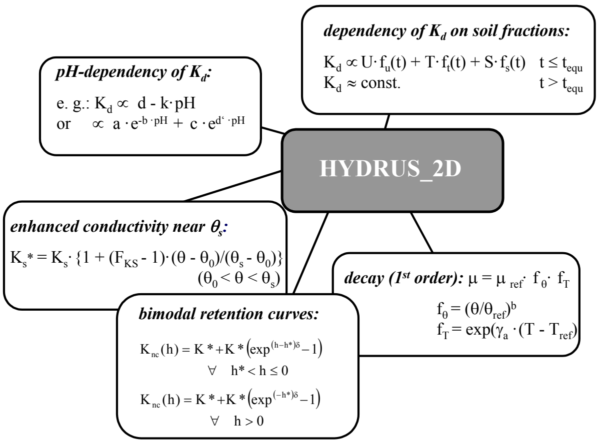


Figure 5: Scheme – Extension of Software as done for HYDRUS_2D

CONCLUSIONS

Deterministic simulation of water and solute transport in the vadose zone contributes to the understanding of natural physical processes. The complex environmental conditions need a good analysis of what will be simulated and which model (concept) is the most appropriate one. With a good background knowledge limitations may be overcome and also misinterpretation is avoidable. The successful run of a simulation does not necessarily prove that the obtained results are correct. Simulation results also contribute to a better interpretation of field measurements, hence the symbiosis between measurement and simulation could be shown .

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BIOGRAPHY

WILLIBALD LOISKANDL, was born in a small village near Vienna, Austria. After a training and some years of professional electrical engineering experience, he studied at the University of Agricultural Sciences Vienna where he obtained his MSc degree 1984 and the PhD in 1988. He also participated in a postgraduate programme in computational hydraulics at the IHE. Delft NL. Since 1984 he belongs to the staff of the university and 1998 he obtained the professorship. Main activities in lecturing are related to hydraulics and soil physics. Research interest are focused on movement of water and solute in the unsaturated zone, modelling and measurement a like.