SIMULATION OF WATER AND SOLUTE TRANSPORT IN UNSATURATED SOILS BY TAKING THE EXAMPLE OF DECENTRALISED TREATED WASTEWATER INFILTRATION

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Abstract

Until the end of 2011 more than 1.7 million small sewage treatment plants in Germany were in operation. By 2015 around 400,000 units will be obsolete due to the laying of new sewer systems. For the remaining units other solutions have to be found concerning the disposal of the treated waste water. This study investigates the possibility of infiltrating treated waste water and hence generating artificial groundwater recharge. The new Groundwater Directive 2006/118/EG requires that the EU member States should implement measures of groundwater protection with the aim of achieving good chemical status of all water bodies by 2015.

Small wastewater treatment plants (SWTP) are a good alternative at sites where no centralized wastewater treatment is available. An effective solution of disposing the treated wastewater by SWTP is direct seepage through the unsaturated soil zone. Climatic and hydrogeological conditions have to be regarded in order to ensure additional purification of the seepage water in the soil and to increase the groundwater recharge rate with water of good quality.

In this study the infiltration and treatment capacity of the vadose zone was initially investigated in laboratory column experiments. An experiment with the infiltration into three different soil types (coarse sand, slightly silty sand and medium silty sand) was carried out.
In parallel, the geohydraulic and chemical processes in the vadose zone were investigated using the simulation software PCSiWaPro® (developed at the Technische Universitaet Dresden, Institute of Waste Management and Contaminated Site), which is a 2D computerized leachate forecast advisory system for the unsaturated soil zone. It is combined with a stochastic weather generator. Using PCSiWaPro® 2D models for all the three column tests were built. To contrast measured with calculated values for each model water influx and outflux, as well as water content measurements at known positions were compared. Furthermore the concentration of sulphate and ammonium was investigated for the influx and outflux water of the soil columns. The results of column tests are also used for the validation of additional modules that were integrated into the simulation software and that regard complex chemical processes. The results are furthermore used to calibrate soil parameters for the simulation of later field experiments.

The agreement between measured and calculated values can be described as very good. The differences were minor and are traced back to uncertainties of the soil parameters and the accuracy of laboratory measurements. From the laboratory and simulated results it can be concluded that only in one column test (medium silty sand) degradation of ammonium was detected. In the other experiments no degradation occurred and the concentration of solutes was above the limiting values. Therefore coarse soils like sand and slightly silty sand are not suitable in this case for infiltration of the treated wastewater in the groundwater without using further preliminary treatment steps.

***Key words**: decentralised wastewater treatment, unsaturated soil zone, column tests, simulation, solute transport, artificial groundwater recharge.*

1. INTRODUCTION

According to the German Institute for Standardization DIN-4261 small wastewater treatment plants are defined as wastewater treatment plants for wastewater from domestic use till a volume of 8 m³ per day, which is roughly equivalent to the amount of wastewater produced by 50 residents.
The disposal of decentralized treated wastewater using small wastewater treatment plants is a big challenge, especially in rural regions where neither a sewer system is available nor drainage into a river or a channel is possible.
This study aims to get benefit of the natural soil capacity for the secondary clarification of the fully biological treated wastewater (Fig. 1). This Method could save energy costs and reduce the environmental (air-soil-groundwater) hazard in addition to support the local groundwater balance.
The use of this method has an additional benefit namely the continuous support of the groundwater recharge which could decrease due to climate change. A comparison over the period 1971-1990 and 1991-2005 shows that the annual rainfall at the station Dresden decreased 47 mm (-37 mm in the winter half-year) (REGKLAM, 2009).

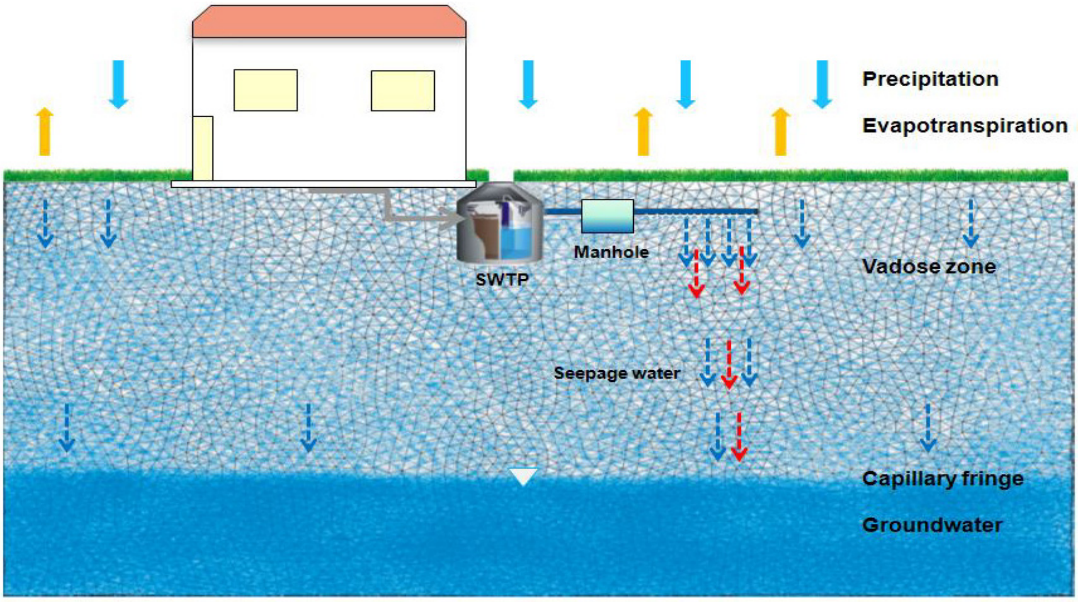

Figure 1. schematical representation of the investigated model and the parameters of soil water balance

There are two possibilities to evaluate the soil clarification capability and the potential hazard for the groundwater either through experimental analysis (on laboratory and field scale) or using suitable modelling programs.
These two evaluation methods will be presented in this study. Therefore three different soil types in the German state Saxony were studied and evaluated.

2. MATERIALS AND METHODS

One of the commonly used means for the investigation of water flow and solute transport processes are laboratory column experiments. This paper presents a comparison between the measured values, infiltration rate and concentration of solutes in the drainage water, using column experiments, and the numerically computed values using the simulation program PCSiWaPro®.

2.1. Theoretical background of the simulation programme PCSiWaPro®

PCSiWaPro® is 2D computerized leachate forecast advisory system for the vadose zone and uses the Finite-Elements Method to solve Richard's equation. The software is a decision support

system developed by the Technical University of Dresden in cooperation with partners from practice which serves as a tool for risk assessment (Graeber, 2006). The program based on the commonly used simulation code SWMS_2D (Šimunek *et al.*, 1994). The simulation program PCSiWaPro® is able to compute the 2D vertical plane and rotationally symmetric flow and transportation processes including the degradation and sorption in the un-/saturated zone. An implemented weather generator simulates the time series of precipitation, solar radiation and evapotranspiration (Nitsch *et al.*, 2007). A soil database is also implemented in PCSiWaPro®.
The flow model using the simulation program PCSiWaPro® describes the vertical flow in the unsaturated zone and it is given by the Richards equation (RE). RE is a standard, frequently used approach for modelling flow in variably saturated porous media (Miller *et al.*, 2005). RE is obtained by combining Darcy's law (equation (2)) with the mass conservation or continuity equation (equation (1)), under the assumption that the air phase remains at constant (atmospheric) pressure and the water phase is uncompressible (Koorevaar *et al.*, 1983). RE is a highly nonlinear partial differential equation that can be cast in several forms, depending on whether pressure (h-based form), moisture (θ-based form), or both (mixed form) are used as state variables (Arampatzis *et al.*, 2001).

$$q = -k\frac{\partial H}{\partial z} = -k\frac{\partial (h+z)}{\partial z} = -k\left(\frac{\partial h}{\partial z}+1\right) \tag{1}$$

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \pm s \tag{2}$$

where q is Flux density ($m^3\ m^{-2} s^{-1}$); H is Head equivalent of hydraulic potential (m); K is hydraulic conductivity (ms^{-1}); h is pressure potential (m); z is elevation (positive upward (m); θ is volumetric water content ($m^3\ m^{-3}$); t is time (s); s is sink/source term ($m^3\ m^{-3} s^{-1}$).
Substitution of equation (1) and equation (2) results in the Richards equation (equation (3)): For 2D-flow modelling like in PCSiWaPro the Richards equation is given in the following form:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left[k\ \left(K_{ij}^{A}\frac{\partial h}{\partial x_i} + K_{iz}^{A}\right)\right] - s \tag{3}$$

With θ as the volumetric water content, x_i are the spatial coordinates (x, y, z), h is the capillary pressure head, t is the time, K_{ij}^{A} and K_{iz}^{A} are the components of the dimensionless anisotropy tensor **K** and K is the function of the unsaturated hydraulic conductivity. The variable s represents the sink or source term, which depends on the capillary pressure head in the soil, and in this case is considered as the amount of water which is removed by plant roots. The water content in the medium depends on the capillary pressure head in the pores and can be described using equation (4):

$$\theta_b = A + \frac{\phi - A - B}{\left[1+(\alpha . h_c)^n\right]^{1-\frac{1}{n}}} \tag{4}$$

where A is the function of the residual water content, B the function of the residual air content, Φ is the porosity of the medium (soil), h_c the capillary pressure head in the pores, α scale parameter and n the slope parameter.
Transport of dissolved material (e.g. in soil water) is usually described with the convection-dispersion-equation. For the substance m (mobile and immobile part) this mass balance equation can be written as (one-dimensional in direction r)

$$\underbrace{\frac{\partial}{\partial r}\left(D\cdot\frac{\partial s_{fl,m}}{\partial r}\right)}_{Dispersion} - \underbrace{\frac{\partial(u\cdot s_{fl,m})}{\partial r}}_{Convection} = \underbrace{\frac{\partial s_m}{\partial t}}_{\substack{Storage\\ change}} + \underbrace{\mu_m\cdot s_m + \gamma_m\cdot\theta}_{\substack{degradation\\ (internal\\ reactions)}} - \underbrace{q_m}_{\substack{Sources/\\ Sinks}} \quad (5)$$

With:

r	m_R	Spatial coordinate	$s_{s,m}$	kg/m_R^3	Specific contaminant mass at the solid phase
t	s	Time	u	m_R/s	Average flow rate
θ	m_{fl}^3/m_R^3	Volumetric water content	γ_m	$kg/(m_{fl}^3\cdot s)$	*0*
D	m_R^2/s	Dispersion coefficient	μ_m	s^{-1}	1^{st} order decay constant
s_m	kg/m_R^3	Specific contaminant mass (s_m=$s_{fl,m}$+$s_{s,m}$)	q_m	$kg/(m_R^3\cdot s)$	Source/sink term for substance m
$s_{fl,m}$	kg/m_R^3	Specific contaminant mass in the liquid phase	R,fl,B identify space, fluid ($1\,m_{fl}^3$ = 1.000l) and soil		

Equation (5) is a hyperbolic differential equation which needs both initial and boundary conditions to be solvable. Although it is formally considered a hyperbolic equation, its solution strongly depends on the dominance of the single terms. It only preserves its hyperbolic form if transport mainly occurs through dispersion/diffusion. If convective transport prevails, eq. (5) shows hyperbolic characteristics. If the substance is strongly degraded, eq. (5) becomes a 1st type ordinary differential equation (Zurmuehl, 1994). As an initial condition either the specific substance mass sorbed at the solid phase, or dissolved in the liquid phase needs to be predefined.

2.2. Column experiments

Laboratory experiments have been conducted for better understanding the soil -treatment (ST) processes occurring during infiltration of sewage effluent through permeable media.
The soils columns were carried out at the institute for waste management and contaminated site treatment of the Technische Universitaet Dresden within the project ESEK (development of an integrated system for the construction of small sewage treatment plants), which was funded by the Federal Ministry of Education and Research BMBF under the code number 02WQ1208.
For the purposes of the laboratory experiments three aerobic (unsaturated) soil columns were built with the incorporation of three different soil materials: coarse sand (B4), medium silty sand (B5) and slightly silty sand (B3). The aims of the implementation of the column

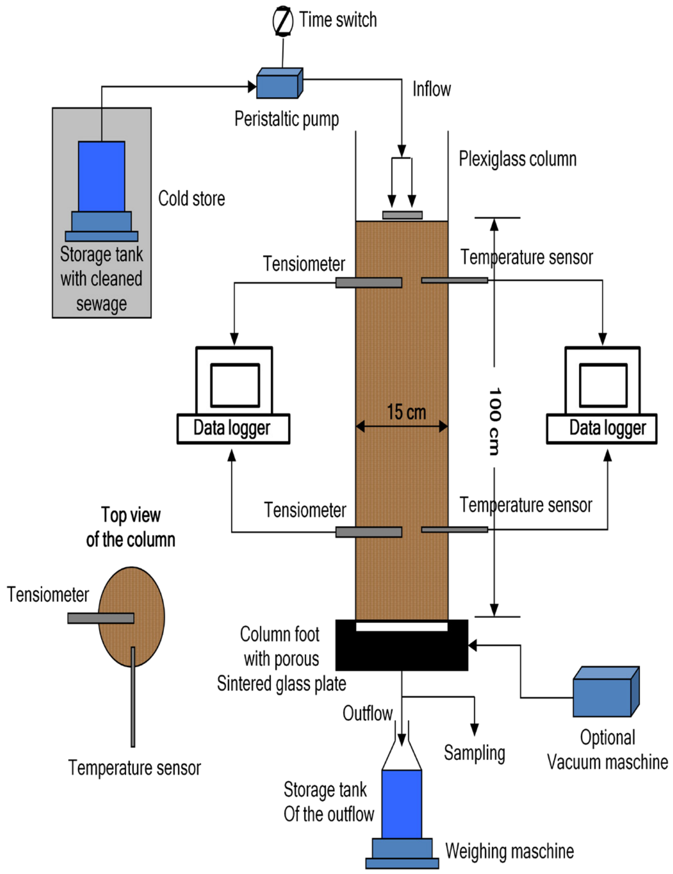

Figure 2. Setup of the soil-column experiment (ESEK, 2011)

experiments are to investigate the effects of different boundary conditions on the infiltration capacity and the cleaning capability of the unsaturated zone. The scheme of the experiment is shown in Figure 2. Transparent Plexiglas columns were used for the experiment, filled with 17663 cm^3 soil (15 cm diameter and 100 cm height), to observe optical effects in the percolation of the waste water. The columns were covered with opaque aluminium foil to prevent biological growth as a result of the incident light, which corresponds to the natural conditions underground. The infiltration boundary of the treated wastewater in the column system is the entire soil surface, whereas the outlet is a free drainage at the bottom of the column. The pumping of the waste water from the reservoir is done by an adjustable peristaltic pump. To determine the amount of infiltrated water the reservoir is located on a scale, so that the flow rate can be determined. Two tensiometers (T) were installed for every column to determine the pressure head. The recording of the measured data for both parameters in a freely selectable time interval is implemented by a data logger.

Within the laboratory experiments, the effects of various conditions on the infiltration as well as the cleaning behaviour of the unsaturated zone in the column experiment were evaluated.

The treated wastewater, which was infiltrated in the soil columns, was taken from a 4EW-SWTP designed for 4 inhabitants. The chosen SWTP bases on the principle of the WSB-technique (Bergmann, 2005).

To suite the seepage to reality changing intervals of the water supply were realized through increased wastewater flow in the morning and evening hours. Figure 3 shows both the laboratory column and for PCSiWaPro® the input infiltration rates and intervals distributed through the day for the three soil types used (B3, B4 and B5).

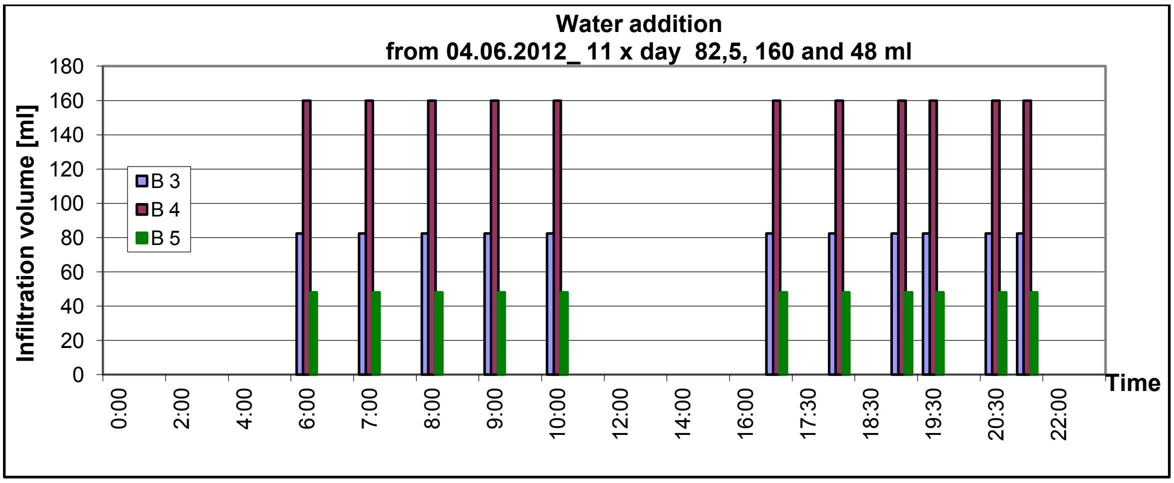

Figure 3. Infiltration rates of sewage for the three investigated soils B3, B4 and B5

3. MODEL SETUP AND SIMULATION BY MEANS OF PCSIWAPRO®

The main steps for the Modelling using this software are the specification of soil and solute parameters, time steps, boundary and initial conditions.

The implemented soil parameters are shown in Tab.1. The required soil hydraulic parameters, could be determined using various sources of information, such as (Busch, et al., 1993), (Kemmesies, 1995), (DIN4220, 2008), and also on the basis of the tracer measurements as well as laboratory experiments.

Table 1 Soil parameters.

Soil type		B3 (slightly silty sand)	B4 (coarse sand)	B5 (medium silty sand)
Porosity *Φ* [-] (determined)		0.44	0.30	0.38
Conductivity K_f [$m.s^{-1}$] (determined)		$5*10^{-5}$	$5*10^{-4}$	$5*10^{-5}$
Residual water content		0.02	0	0.03
Van–Genuchten Parameters (DIN 4220)	n	1.23	1.47	1.21
	m	0.19	0.32	0.17
	λ	0.5	0.5	0.5
	α_d	0.204	0.221	0.089
	α_i	0.408	0.442	0.178
Bulk density [g/cm^3] (estimated)		1.492	1.859	1.650

The infiltration rates were defined as the upper boundary condition of the column-model. Since PCSiWaPro® is a 2D-modelling-software the added wastewater in the lab should be converted according to the defined cross-section of the column (Hasan et al., 2012), e.g. for B3 82.5 ml/feed corresponds 0.47 cm/feed (1 feed=15 minutes) after the conversion.

The lower boundary condition of the model was defined as a seepage face, which means that the seepage water can flow out of the defined model body only after the full saturation of the boundary. The modelling using PCSiWaPro® requires also the specification of the initial condition for the flow calculation. For numerical models, it is generally recommended to specify initial conditions in as pressure head, since this variable is the driving force for water flow. Specifying initial conditions in terms of the water content often leads to unrealistically large pressure head gradients and, consequently, water fluxes across textural boundaries, after water contents are converted into pressure heads using the soil water retention curves (Simunek et al., 2010).
The implemented initial pressure heads for the studied soil columns vary from -20 cm (for B5) to -50 cm (for B4).
The average input concentrations of So_4^{-2} and NH_4^+, which were determined in the treated wastewater used for the infiltration in the laboratory, are 125 mg/l and 26 mg/l respectively. These values are the same for the three soil types since the same source of sewage was used.

The most relevant step to simulate the solute transport is to put in the soil specific, sorption and reactive (degradation) parameters. In case of sulphate transport the very low sorption and the non-occurred degradation processes weren't regarded. Therefore, the main considered processes were diffusion, dispersion and advection. Ammonium is a well degradable and an absorbable ion. That requires the consideration of all potential transport processes. The decay constant first order of Ammonium, at B5, was for example -0.0125 min-^{1}.

(The last step of the actual modelling is the simulation process. Figure 5 shows the graphical display during the simulation run, which allowed a first assessment of the results. During the simulation run at custom times, different information (pressure heads, water content, saturation degree, concentration, etc.) of all nodes and in particular to the conditions in an output database could be shown.)

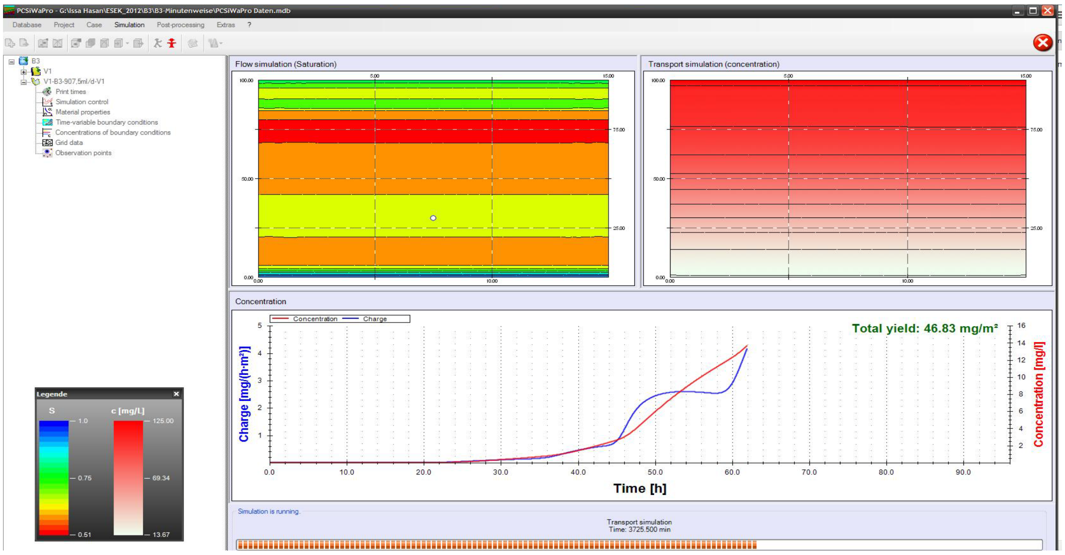

Figure 4. Simulations run at the interface of PCSiWaPro®

4. RESULTS AND DISCUSSION

The installed experiments and the related models achieved to prevent full saturation conditions in the studied soils to enable aerobic biological degradation processes, which lead to a decline in the solute concentrations and consequently to the purification of infiltrated wastewater through the vadose zone into the groundwater. The distribution of the water saturation varies as expected according to the soil type and B4 was clearly drier than both B3 and B5, because of its higher hydraulic conductivity and lower storage capacity, and the three soils were all the experiments time, as required, under unsaturated conditions (see Fig. 5).

In spite of the parameter assumption according to the available database without an accurate estimation a clear agreement between measured and computed outfluxes (drainage rates) and pressure heads (water retention) could be achieved (Fig. 6). To observe the change of the water content or the pressure head two observation points were integrated for every column-model respective to the position of the lab-tensiometers. This comparison with measured data is the common method to validate software. After a successful validation the computation of further case studies can be conducted.

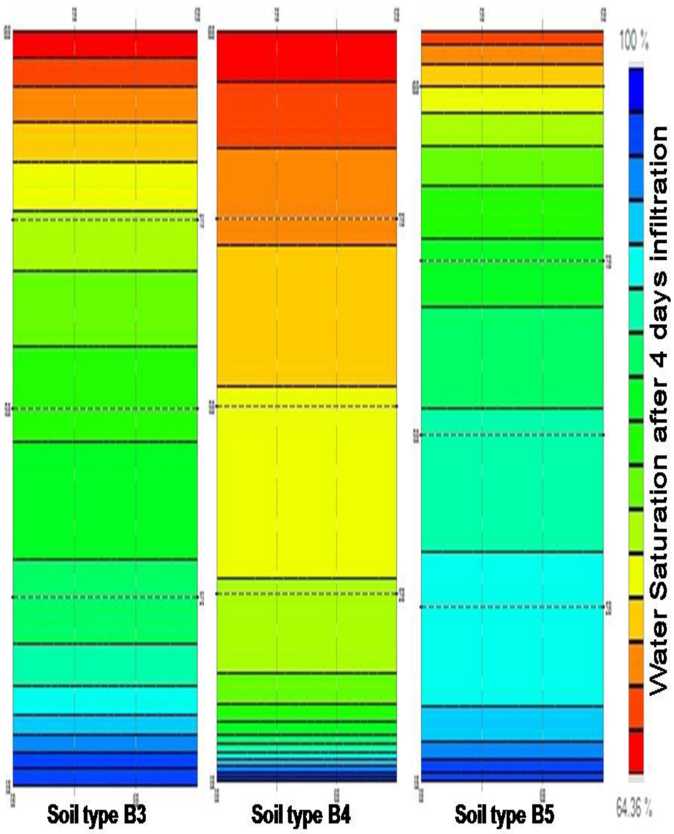

Figure 5. Distribution of water saturation after 4 days of infiltration for the investigated soils

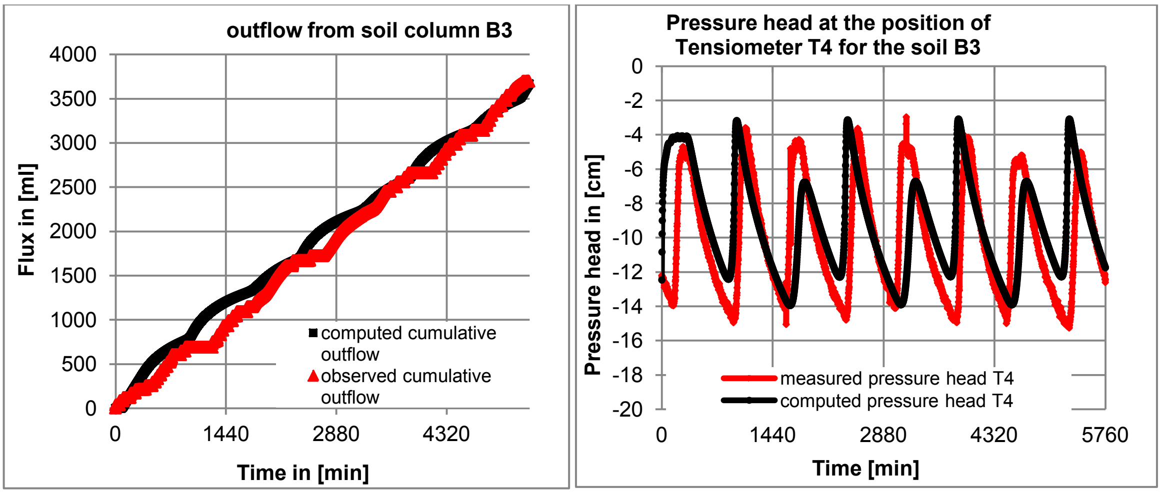

Figure 6. Comparison between measured and computed values (drain water (outflow), pressure head) for B3

The recent laboratory results of leaching experiments regarding treated wastewater infiltration are presented in Figure 7. The concentration of sulphate (approximately 125 mg/l) in the inlets and outlets for the investigated soil columns shows no change during the simulations and experiments time; this is because of the nonexistent sorption and degradation terms. Colmatation or Clogging effects were not observed in all experimental columns. The reason for this is certainly the small amount of filterable substances in treated effluents. The decay of the infiltrated wastewater for the soils B3 and B4 despite a reduced amount of water remained incomplete and isn't insufficient for wastewater infiltration in case of near-surface groundwater levels. The reason is the strong sinking pH-value during the passage of water through the soil columns, which could indicate that these two soils have low puffer capacities. Thus the conditions for aerobic biological degradation processes in the soil are not optimal. Soil B5 had by contrast a steady pH-value during the whole experiment time which offers suitable conditions for a complete decay of ammonium in the infiltrated wastewater. Although the soils B3 and B5 have very similar physical properties, the difference in cleaning capability was enormous.

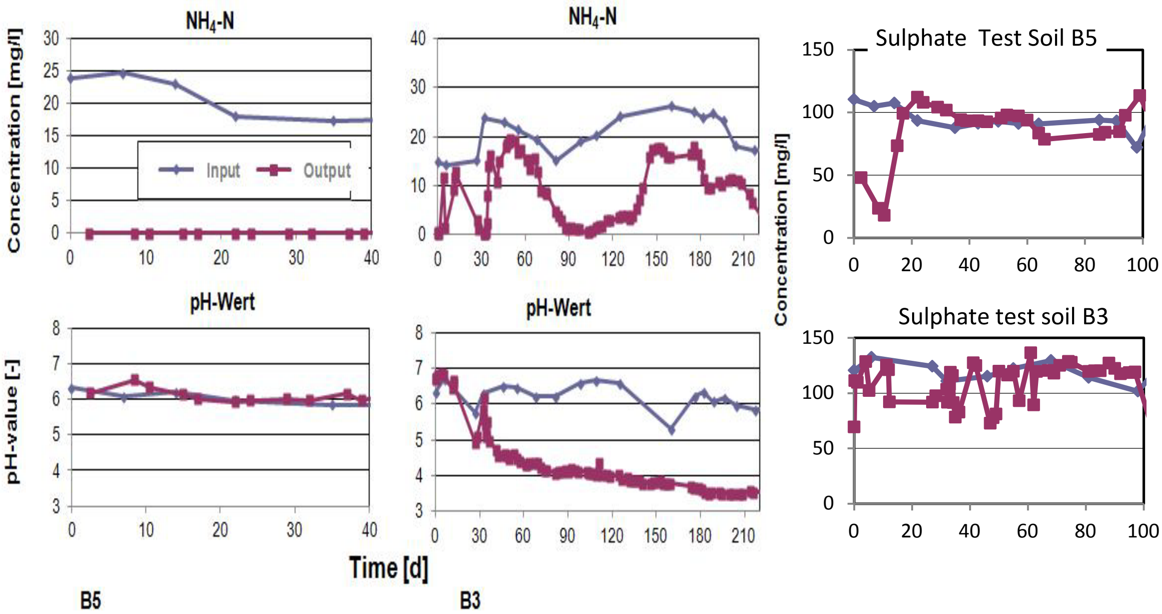

Figure 7. Measured results pH-value and NH_4-N-concentration for the soils B3 and B5 (left) and sulphate analysis for B5 and B3 (right)

With the aid of PCSiWaPro® it is possible to simulate decay of 0. and 1. order. Returning to the laboratory results for soil B5 it is clear that the occurred decay in this case is 1.order.

Figure 8 shows the comparison of Ammonium-concentration at the outlet of the three related soil columns B3, B4 and B5. The simulated concentration of ammonium in the outlet of the soil column B5 was nearly zero (compare fig. 7 with fig. 8). The ammonium ions take at B5 about 3.5 days to reach the bottom of the column (transport velocity = $3*10^{-6}$ $m.s^{-1}$). At B3 and B4 no decay had taken place (fig. 8).

The obtained results could then be implemented for the simulation on field scale under consideration of the highest anticipated depth of the water table, which should be in any case≥ 0.6 m from the sole of the infiltration system / sole grave (SaechsWG, 2009)

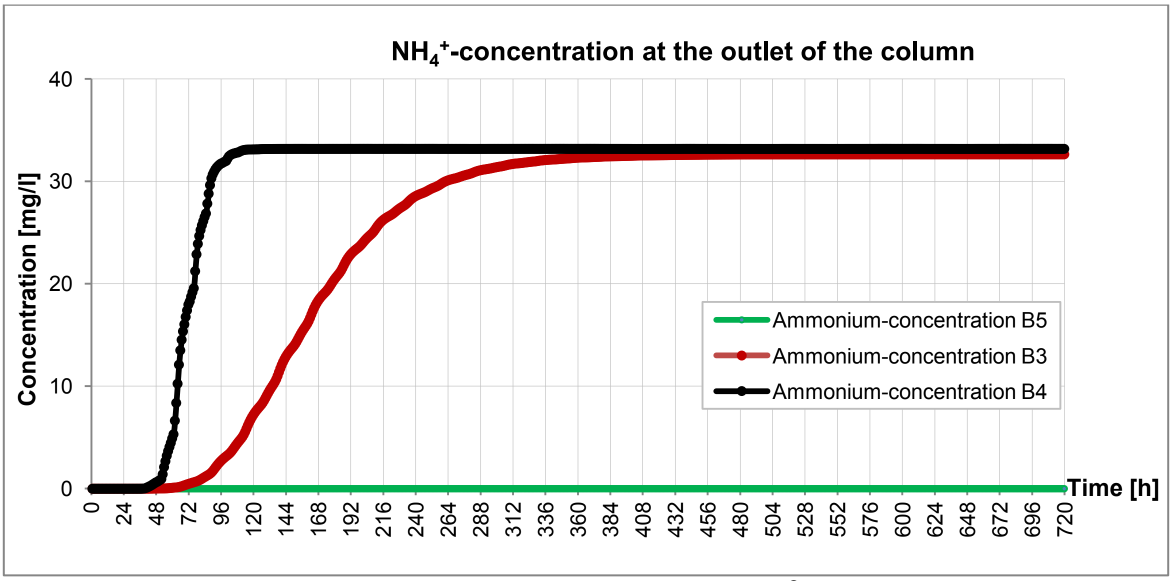

Figure 8. Computed Ammonium- concentration using PCSiWaPro® for the three studied soils B3, B4 and B5 during 30 days of simulation

5. CONCLUSIONS AND RECOMMENDATIONS

The agreement between simulation measured results of both water balance and solute transport was very good in the three studied cases B3, B4 and B5. The slight variation attributes mainly to the uncertainties of the soil parameters (due to insufficient data). The applicability of a model depends in general on how closely the mathematical equations approximate the physical system being modelled. Because of the simplifying assumptions embedded in the mathematical equations and the many uncertainties in the values of data required by the model, a model must be viewed as an approximation and not an exact duplication of field conditions. The achieved accordance confirms the succeeded validation of the program PCSiWaPro®.

Colmatation or Clogging effects in the three investigated experimental columns could not be observed due to the small amount of suspended solids in the infiltrated wastewater. Based on the study results it can be stated that the infiltration of decentralised treated wastewater in the soil could only be allowed after the physical and chemical analysis of the destination soil, because only certain kinds of soil are suitable for this technique of purification (e.g. B5).

The aim of further work is the development of the program PCSiWaPro® to enable the inverse solution for the calibration of the solute and soil parameters on the basis of observed data for a more accurate simulation results and to consider not only the single solutes but rather their interactions. The presented results in this study show that even for physically similar soil types the transport processes and especially the degradation processes are enormously different. Therefore it is necessary that in addition to soil physics analysis, which is the criterion for the infiltration capacity of the soil, also a chemical analysis of the soil and transformation experiments of the studied solutes are be carried out.

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